



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 12:21 AM UTC

PDB ID : 3BTU / pdb_00003btu
Title : Crystal structure of the super-repressor mutant of Gal80p from *Saccharomyces cerevisiae*; Gal80(S2) [E351K]
Authors : Kumar, P.R.; Joshua-Tor, L.
Deposited on : 2007-12-30
Resolution : 2.85 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

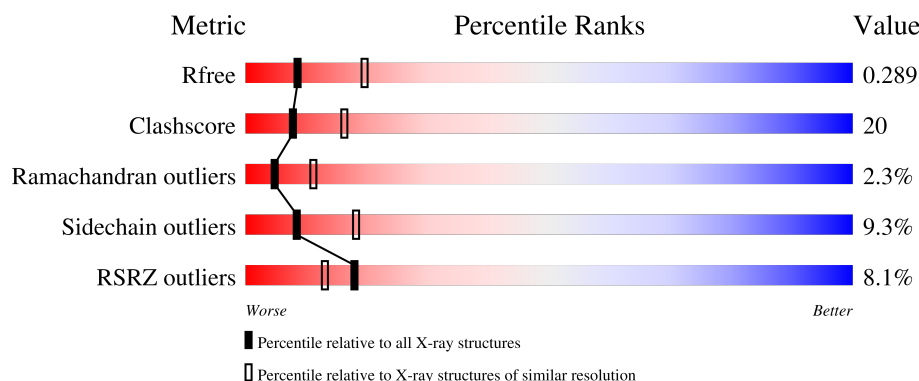
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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}	180053	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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 $\leq 5\%$. 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	438	
1	B	438	
1	C	438	
1	D	438	
1	E	438	

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Mol	Chain	Length	Quality of chain
1	F	438	14% 46% 36% 5% 12%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 18389 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 Galactose/lactose metabolism regulatory protein GAL80.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	0	0
			3088	1987	518	572	11			
1	B	389	Total	C	N	O	S	0	0	0
			3065	1975	513	566	11			
1	C	388	Total	C	N	O	S	0	0	0
			3057	1969	511	566	11			
1	D	392	Total	C	N	O	S	0	0	0
			3087	1987	518	571	11			
1	E	387	Total	C	N	O	S	0	0	0
			3046	1960	512	563	11			
1	F	387	Total	C	N	O	S	0	0	0
			3046	1960	512	563	11			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P04387
A	-1	SER	-	expression tag	UNP P04387
A	0	HIS	-	expression tag	UNP P04387
A	351	LYS	GLU	engineered mutation	UNP P04387
B	-2	GLY	-	expression tag	UNP P04387
B	-1	SER	-	expression tag	UNP P04387
B	0	HIS	-	expression tag	UNP P04387
B	351	LYS	GLU	engineered mutation	UNP P04387
C	-2	GLY	-	expression tag	UNP P04387
C	-1	SER	-	expression tag	UNP P04387
C	0	HIS	-	expression tag	UNP P04387
C	351	LYS	GLU	engineered mutation	UNP P04387
D	-2	GLY	-	expression tag	UNP P04387
D	-1	SER	-	expression tag	UNP P04387
D	0	HIS	-	expression tag	UNP P04387
D	351	LYS	GLU	engineered mutation	UNP P04387
E	-2	GLY	-	expression tag	UNP P04387

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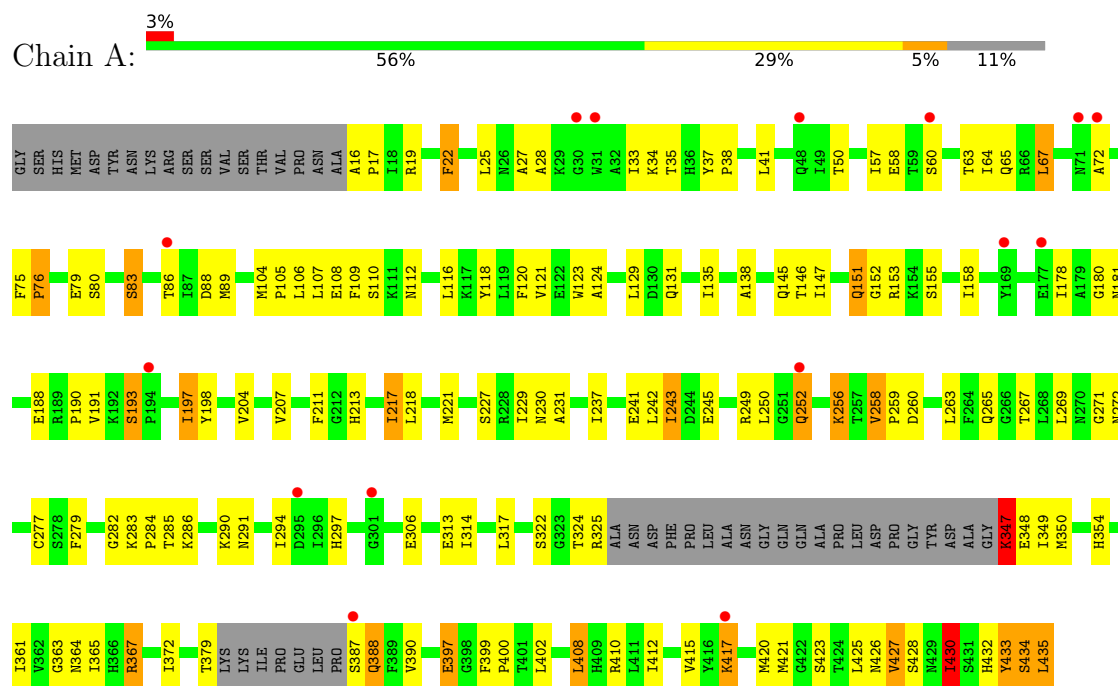
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Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	SER	-	expression tag	UNP P04387
E	0	HIS	-	expression tag	UNP P04387
E	351	LYS	GLU	engineered mutation	UNP P04387
F	-2	GLY	-	expression tag	UNP P04387
F	-1	SER	-	expression tag	UNP P04387
F	0	HIS	-	expression tag	UNP P04387
F	351	LYS	GLU	engineered mutation	UNP P04387

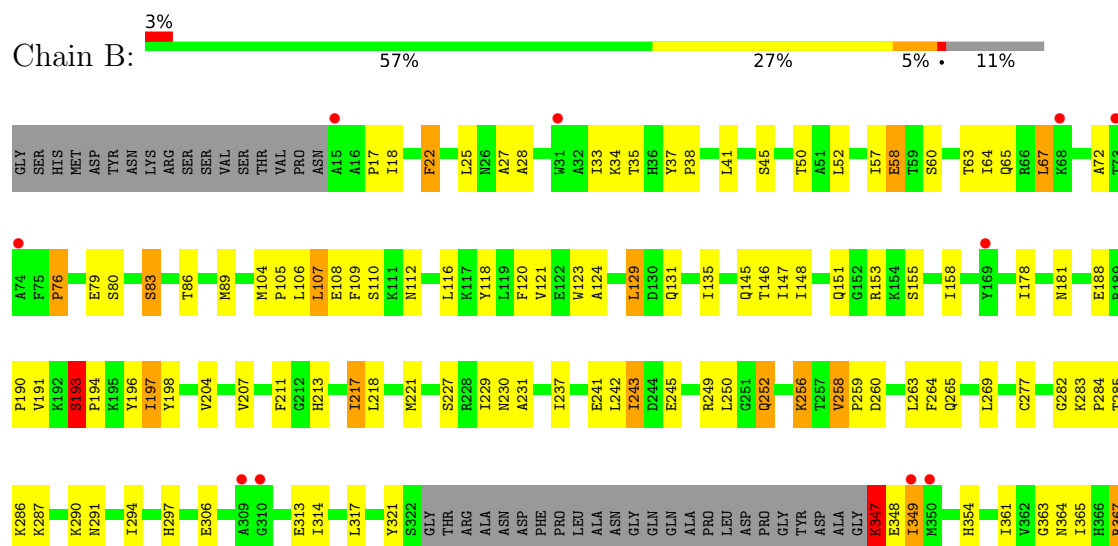
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Galactose/lactose metabolism regulatory protein GAL80

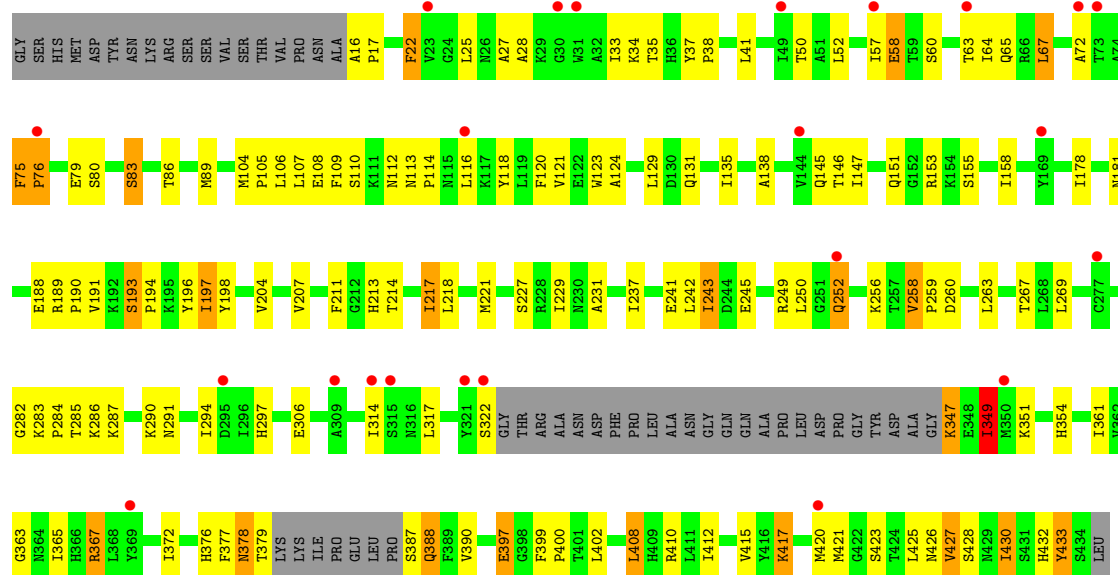


- Molecule 1: Galactose/lactose metabolism regulatory protein GAL80

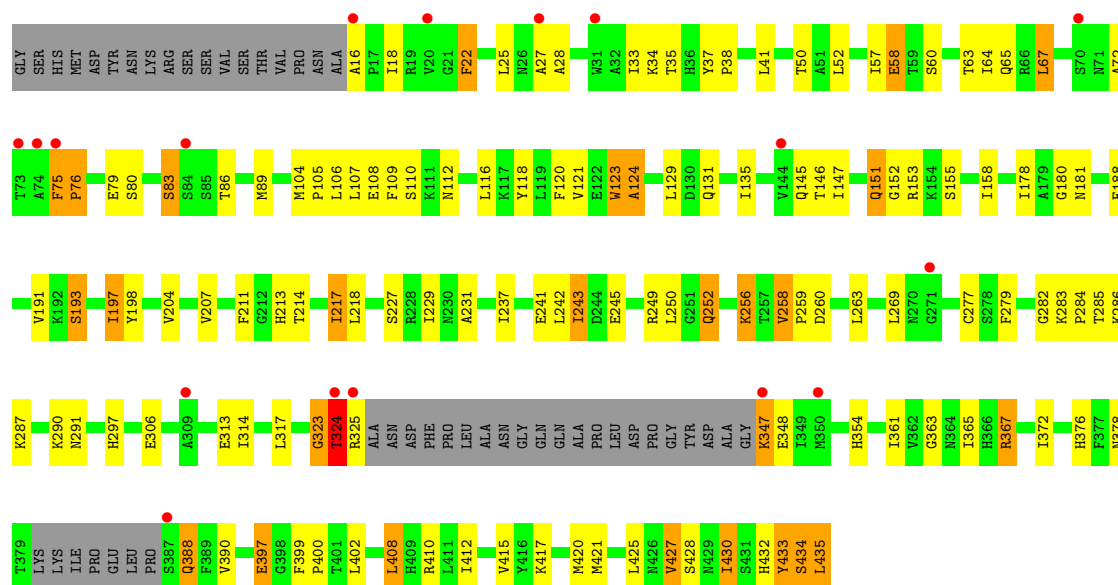




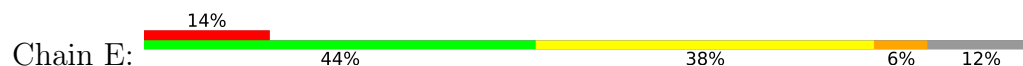
- Molecule 1: Galactose/lactose metabolism regulatory protein GAL80

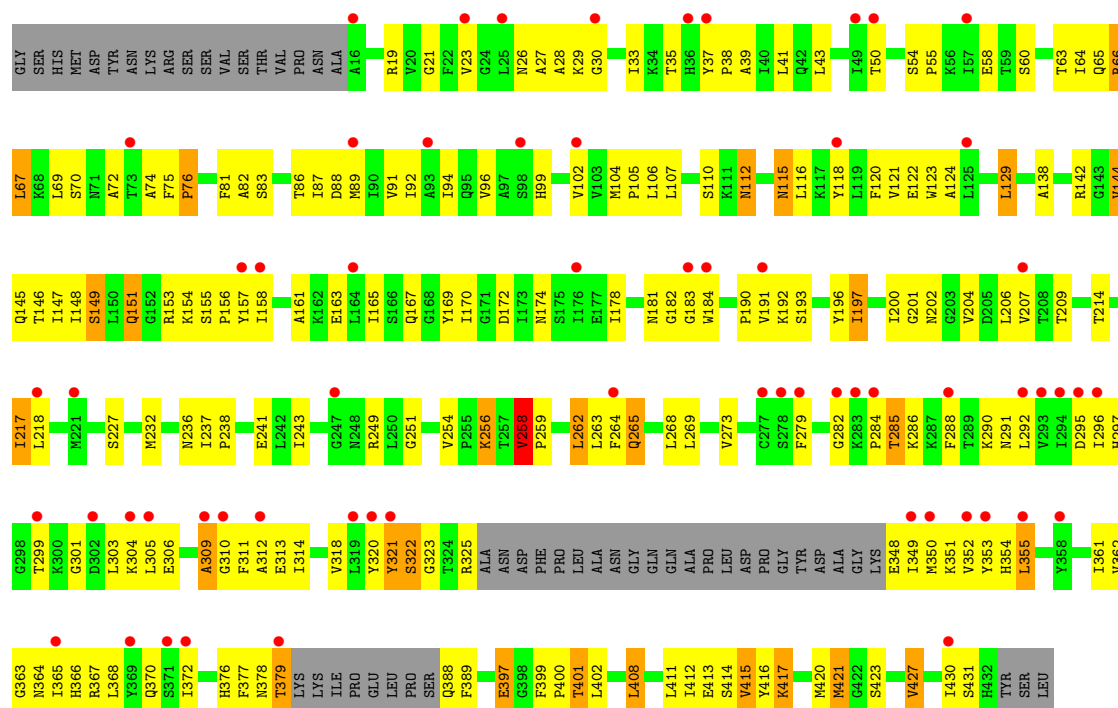


- Molecule 1: Galactose/lactose metabolism regulatory protein GAL80

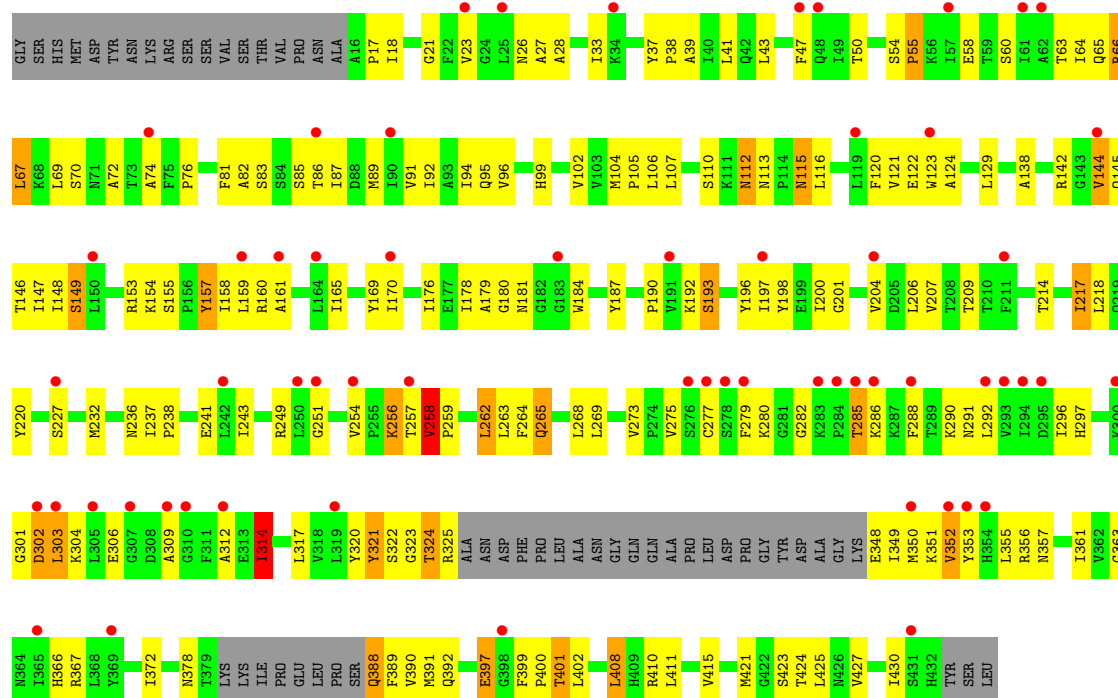


- Molecule 1: Galactose/lactose metabolism regulatory protein GAL80





● Molecule 1: Galactose/lactose metabolism regulatory protein GAL80



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	495.32Å 84.86Å 66.46Å 90.00° 98.90° 90.00°	Depositor
Resolution (Å)	50.00 – 2.85 50.00 – 2.85	Depositor EDS
% Data completeness (in resolution range)	85.6 (50.00-2.85) 85.6 (50.00-2.85)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.2.0019, PHENIX	Depositor
R, R_{free}	0.228 , 0.278 0.249 , 0.289	Depositor DCC
R_{free} test set	5498 reflections (8.48%)	wwPDB-VP
Wilson B-factor (Å ²)	66.4	Xtriage
Anisotropy	0.629	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 72.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.040 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	18389	wwPDB-VP
Average B, all atoms (Å ²)	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% 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, 0.333 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	0.43	0/3155	0.80	6/4270 (0.1%)
1	B	0.43	0/3132	0.82	4/4240 (0.1%)
1	C	0.43	0/3124	0.82	6/4230 (0.1%)
1	D	0.45	0/3154	0.82	8/4270 (0.2%)
1	E	0.36	0/3112	0.77	2/4214 (0.0%)
1	F	0.35	0/3112	0.75	2/4214 (0.0%)
All	All	0.41	0/18789	0.80	28/25438 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	347	LYS	N-CA-C	-10.23	82.37	111.00
1	B	347	LYS	N-CA-C	-9.98	83.05	111.00
1	D	323	GLY	N-CA-C	8.04	121.29	110.43
1	C	379	THR	N-CA-C	-6.41	93.06	111.00
1	F	258	VAL	CA-C-N	5.95	125.89	119.76
1	F	258	VAL	C-N-CA	5.95	125.89	119.76
1	B	193	SER	CA-C-N	5.84	126.14	119.83
1	B	193	SER	C-N-CA	5.84	126.14	119.83
1	B	321	TYR	N-CA-C	5.82	117.61	107.49
1	A	347	LYS	N-CA-C	-5.70	95.06	111.00
1	D	75	PHE	CA-C-N	5.53	126.75	119.84
1	D	75	PHE	C-N-CA	5.53	126.75	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	258	VAL	CA-C-N	5.41	125.33	119.76
1	E	258	VAL	C-N-CA	5.41	125.33	119.76
1	C	193	SER	CA-C-N	5.34	125.60	119.83
1	C	193	SER	C-N-CA	5.34	125.60	119.83
1	D	193	SER	CA-C-N	5.30	125.55	119.83
1	D	193	SER	C-N-CA	5.30	125.55	119.83
1	C	75	PHE	CA-C-N	5.24	126.39	119.84
1	C	75	PHE	C-N-CA	5.24	126.39	119.84
1	D	16	ALA	CA-C-N	5.15	125.08	119.78
1	D	16	ALA	C-N-CA	5.15	125.08	119.78
1	A	348	GLU	N-CA-C	5.11	116.63	108.41
1	D	434	SER	N-CA-C	-5.06	108.13	114.56
1	A	75	PHE	CA-C-N	5.04	126.15	119.84
1	A	75	PHE	C-N-CA	5.04	126.15	119.84
1	A	193	SER	CA-C-N	5.03	125.26	119.83
1	A	193	SER	C-N-CA	5.03	125.26	119.83

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	123	TRP	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3088	0	3101	112	0
1	B	3065	0	3080	111	0
1	C	3057	0	3067	116	0
1	D	3087	0	3101	109	0
1	E	3046	0	3058	169	0
1	F	3046	0	3058	160	0
All	All	18389	0	18465	734	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 20.

All (734) 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:D:347:LYS:N	1:D:348:GLU:CA	1.70	1.34
1:E:155:SER:HB3	1:E:158:ILE:HD13	1.41	1.03
1:B:347:LYS:HD2	1:B:347:LYS:O	1.59	0.99
1:C:349:ILE:HD11	1:C:351:LYS:HE3	1.48	0.94
1:D:347:LYS:N	1:D:348:GLU:HA	0.77	0.92
1:F:427:VAL:HG13	1:F:430:ILE:HG13	1.51	0.92
1:E:263:LEU:HB3	1:F:265:GLN:HE21	1.35	0.91
1:D:347:LYS:O	1:D:347:LYS:HG3	1.72	0.90
1:F:292:LEU:HD21	1:F:312:ALA:HB2	1.55	0.88
1:D:410:ARG:HB3	1:D:430:ILE:HD12	1.53	0.87
1:B:410:ARG:HB3	1:B:430:ILE:HD12	1.57	0.86
1:E:304:LYS:HG2	1:E:305:LEU:H	1.40	0.86
1:A:410:ARG:HB3	1:A:430:ILE:HD12	1.57	0.86
1:E:265:GLN:HE21	1:F:263:LEU:HB3	1.41	0.85
1:C:410:ARG:HB3	1:C:430:ILE:HD12	1.58	0.85
1:E:151:GLN:HG2	1:E:365:ILE:HD13	1.60	0.82
1:E:427:VAL:HG12	1:E:430:ILE:HG13	1.60	0.82
1:B:347:LYS:HD2	1:B:347:LYS:C	2.05	0.82
1:F:361:ILE:HD12	1:F:361:ILE:H	1.45	0.81
1:A:153:ARG:HD2	1:A:400:PRO:HG3	1.63	0.81
1:C:153:ARG:HD2	1:C:400:PRO:HG3	1.63	0.80
1:E:427:VAL:HG12	1:E:430:ILE:CG1	2.13	0.79
1:E:265:GLN:NE2	1:F:263:LEU:HB3	1.97	0.79
1:C:27:ALA:HB1	1:C:67:LEU:HD21	1.65	0.78
1:E:263:LEU:HB3	1:F:265:GLN:NE2	1.98	0.78
1:D:324:THR:HG22	1:D:324:THR:O	1.83	0.78
1:A:417:LYS:HG3	1:C:417:LYS:HZ3	1.47	0.77
1:D:153:ARG:HD2	1:D:400:PRO:HG3	1.66	0.77
1:F:268:LEU:HB2	1:F:273:VAL:HB	1.67	0.77
1:E:258:VAL:HG13	1:E:259:PRO:HD2	1.67	0.77
1:B:27:ALA:HB1	1:B:67:LEU:HD21	1.67	0.77
1:D:27:ALA:HB1	1:D:67:LEU:HD21	1.66	0.76
1:E:268:LEU:HB2	1:E:273:VAL:HB	1.66	0.76
1:C:349:ILE:HD13	1:C:349:ILE:O	1.85	0.76
1:D:89:MET:HE1	1:D:372:ILE:HG21	1.66	0.76
1:A:27:ALA:HB1	1:A:67:LEU:HD21	1.68	0.76
1:A:89:MET:HE1	1:A:372:ILE:HG21	1.68	0.76
1:E:146:THR:HB	1:E:402:LEU:HG	1.67	0.76
1:C:79:GLU:O	1:C:83:SER:HB2	1.86	0.75
1:A:79:GLU:O	1:A:83:SER:HB2	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:79:GLU:O	1:D:83:SER:HB2	1.87	0.75
1:E:145:GLN:HE21	1:E:388:GLN:HG3	1.50	0.75
1:F:206:LEU:HD11	1:F:279:PHE:HB3	1.69	0.74
1:F:258:VAL:HG13	1:F:259:PRO:HD2	1.69	0.74
1:B:153:ARG:HD2	1:B:400:PRO:HG3	1.68	0.74
1:F:176:ILE:HD13	1:F:218:LEU:HD11	1.70	0.74
1:E:376:HIS:HD2	1:E:377:PHE:CE1	2.06	0.74
1:E:145:GLN:NE2	1:E:388:GLN:HG3	2.01	0.74
1:C:50:THR:HG21	1:C:86:THR:HB	1.69	0.73
1:B:79:GLU:O	1:B:83:SER:HB2	1.87	0.73
1:B:50:THR:HG21	1:B:86:THR:HB	1.69	0.73
1:E:206:LEU:HD11	1:E:279:PHE:HB3	1.69	0.73
1:E:292:LEU:HD21	1:E:312:ALA:HB2	1.71	0.73
1:F:352:VAL:HG12	1:F:353:TYR:N	2.03	0.73
1:B:89:MET:HE1	1:B:372:ILE:HG21	1.70	0.73
1:C:89:MET:HE1	1:C:372:ILE:HG21	1.71	0.72
1:F:64:ILE:HG23	1:F:72:ALA:HB3	1.71	0.72
1:A:57:ILE:HD12	1:A:76:PRO:HA	1.71	0.72
1:A:241:GLU:HG2	1:A:249:ARG:HD3	1.71	0.72
1:B:241:GLU:HG2	1:B:249:ARG:HD3	1.71	0.72
1:D:241:GLU:HG2	1:D:249:ARG:HD3	1.70	0.72
1:E:37:TYR:HB3	1:E:38:PRO:HD3	1.70	0.72
1:E:64:ILE:HG23	1:E:72:ALA:HB3	1.71	0.72
1:F:146:THR:HB	1:F:402:LEU:HG	1.69	0.72
1:D:50:THR:HG21	1:D:86:THR:HB	1.71	0.72
1:C:57:ILE:HD12	1:C:76:PRO:HA	1.70	0.72
1:C:104:MET:HB2	1:C:105:PRO:HD3	1.72	0.72
1:A:50:THR:HG21	1:A:86:THR:HB	1.70	0.72
1:E:170:ILE:HB	1:E:301:GLY:O	1.89	0.72
1:A:104:MET:HB2	1:A:105:PRO:HD3	1.72	0.71
1:C:27:ALA:HB2	1:C:63:THR:HG23	1.73	0.71
1:E:161:ALA:O	1:E:165:ILE:HG13	1.90	0.71
1:D:22:PHE:CD2	1:D:25:LEU:HB2	2.25	0.71
1:C:241:GLU:HG2	1:C:249:ARG:HD3	1.71	0.71
1:D:57:ILE:HD12	1:D:76:PRO:HA	1.71	0.71
1:B:104:MET:HB2	1:B:105:PRO:HD3	1.72	0.70
1:D:131:GLN:O	1:D:135:ILE:HG13	1.90	0.70
1:E:157:TYR:OH	1:E:355:LEU:HB2	1.92	0.70
1:A:397:GLU:CD	1:A:397:GLU:H	2.00	0.70
1:B:22:PHE:CD2	1:B:25:LEU:HB2	2.27	0.70
1:D:104:MET:HB2	1:D:105:PRO:HD3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:297:HIS:NE2	1:F:286:LYS:HD3	2.06	0.70
1:C:285:THR:HB	1:C:291:ASN:HD21	1.57	0.70
1:E:288:PHE:CE2	1:F:320:TYR:HB3	2.26	0.70
1:B:27:ALA:HB2	1:B:63:THR:HG23	1.74	0.69
1:F:37:TYR:HB3	1:F:38:PRO:HD3	1.73	0.69
1:B:57:ILE:HD12	1:B:76:PRO:HA	1.75	0.69
1:B:397:GLU:CD	1:B:397:GLU:H	2.01	0.69
1:C:131:GLN:O	1:C:135:ILE:HG13	1.92	0.69
1:F:352:VAL:HG12	1:F:353:TYR:H	1.56	0.69
1:C:377:PHE:O	1:C:378:ASN:C	2.36	0.69
1:F:83:SER:OG	1:F:112:ASN:HB2	1.93	0.68
1:C:397:GLU:CD	1:C:397:GLU:H	2.01	0.68
1:C:22:PHE:CD2	1:C:25:LEU:HB2	2.29	0.68
1:B:131:GLN:O	1:B:135:ILE:HG13	1.94	0.67
1:A:22:PHE:CD2	1:A:25:LEU:HB2	2.29	0.67
1:E:83:SER:OG	1:E:112:ASN:HB2	1.95	0.67
1:E:207:VAL:HG22	1:E:262:LEU:HD22	1.77	0.67
1:A:158:ILE:HG12	1:A:217:ILE:HG21	1.77	0.67
1:A:27:ALA:HB2	1:A:63:THR:HG23	1.76	0.66
1:C:145:GLN:HE21	1:C:388:GLN:HG3	1.58	0.66
1:E:155:SER:HA	1:E:364:ASN:ND2	2.10	0.66
1:F:67:LEU:O	1:F:69:LEU:HG	1.95	0.66
1:D:237:ILE:O	1:D:256:LYS:NZ	2.26	0.66
1:E:67:LEU:O	1:E:69:LEU:HG	1.96	0.66
1:E:145:GLN:HE22	1:E:389:PHE:H	1.44	0.66
1:A:131:GLN:O	1:A:135:ILE:HG13	1.96	0.65
1:D:123:TRP:CH2	1:D:408:LEU:HD13	2.30	0.65
1:D:27:ALA:HB2	1:D:63:THR:HG23	1.78	0.65
1:A:285:THR:HB	1:A:291:ASN:HD21	1.62	0.65
1:F:153:ARG:HD2	1:F:400:PRO:HG3	1.77	0.65
1:B:178:ILE:HD11	1:B:218:LEU:HD22	1.77	0.65
1:D:397:GLU:CD	1:D:397:GLU:H	2.02	0.65
1:D:158:ILE:HG12	1:D:217:ILE:HG21	1.78	0.64
1:B:158:ILE:HG12	1:B:217:ILE:HG21	1.79	0.64
1:A:363:GLY:O	1:A:367:ARG:HD2	1.97	0.64
1:E:286:LYS:HD3	1:F:297:HIS:NE2	2.12	0.64
1:B:227:SER:HB2	1:B:269:LEU:HD12	1.80	0.64
1:C:349:ILE:CD1	1:C:351:LYS:HE3	2.24	0.64
1:F:207:VAL:HG22	1:F:262:LEU:HD22	1.79	0.64
1:F:322:SER:HB2	1:F:350:MET:HG2	1.79	0.64
1:F:352:VAL:CG1	1:F:353:TYR:H	2.10	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:256:LYS:HE2	1:F:258:VAL:O	1.98	0.64
1:C:158:ILE:HG12	1:C:217:ILE:HG21	1.79	0.64
1:F:123:TRP:CD2	1:F:124:ALA:N	2.64	0.63
1:B:285:THR:HB	1:B:291:ASN:HD21	1.63	0.63
1:C:237:ILE:O	1:C:256:LYS:NZ	2.29	0.63
1:D:285:THR:HB	1:D:291:ASN:HD21	1.62	0.63
1:E:21:GLY:HA3	1:E:87:ILE:HD13	1.80	0.63
1:F:123:TRP:CG	1:F:124:ALA:H	2.16	0.63
1:E:43:LEU:HD11	1:E:366:HIS:CD2	2.33	0.63
1:E:408:LEU:O	1:E:412:ILE:HG12	1.99	0.63
1:E:142:ARG:HG3	1:E:144:VAL:HG13	1.81	0.63
1:D:123:TRP:CG	1:D:124:ALA:N	2.66	0.63
1:E:123:TRP:CG	1:E:124:ALA:H	2.16	0.63
1:B:347:LYS:C	1:B:347:LYS:CD	2.72	0.62
1:E:389:PHE:HE1	1:E:401:THR:CG2	2.13	0.62
1:F:262:LEU:HD12	1:F:263:LEU:O	2.00	0.62
1:E:120:PHE:HZ	1:E:368:LEU:HD23	1.65	0.62
1:E:303:LEU:HD23	1:E:304:LYS:N	2.15	0.62
1:A:297:HIS:CE1	1:B:286:LYS:HD3	2.35	0.62
1:F:123:TRP:CG	1:F:124:ALA:N	2.67	0.62
1:D:363:GLY:O	1:D:367:ARG:HD2	2.00	0.62
1:B:290:LYS:HG3	1:B:306:GLU:HB3	1.80	0.62
1:D:427:VAL:HG13	1:D:427:VAL:O	2.00	0.62
1:F:142:ARG:HG3	1:F:144:VAL:HG13	1.82	0.61
1:A:290:LYS:HG3	1:A:306:GLU:HB3	1.82	0.61
1:E:313:GLU:HG2	1:E:314:ILE:HG23	1.82	0.61
1:F:21:GLY:HA3	1:F:87:ILE:HD13	1.81	0.61
1:D:434:SER:O	1:D:435:LEU:HD22	2.00	0.61
1:F:145:GLN:HE21	1:F:388:GLN:HG3	1.65	0.61
1:A:347:LYS:HE3	1:A:347:LYS:HA	1.82	0.61
1:C:297:HIS:NE2	1:D:286:LYS:HD3	2.16	0.61
1:D:178:ILE:HD11	1:D:218:LEU:HD22	1.83	0.61
1:A:146:THR:HB	1:A:402:LEU:HG	1.82	0.60
1:D:145:GLN:HE21	1:D:388:GLN:HG3	1.65	0.60
1:E:123:TRP:CG	1:E:124:ALA:N	2.68	0.60
1:E:320:TYR:HB3	1:F:288:PHE:CE2	2.36	0.60
1:F:321:TYR:CG	1:F:321:TYR:O	2.54	0.60
1:F:352:VAL:CG1	1:F:353:TYR:N	2.64	0.60
1:C:178:ILE:HD11	1:C:218:LEU:HD22	1.81	0.60
1:E:26:ASN:O	1:E:33:ILE:HB	2.02	0.60
1:A:123:TRP:CD2	1:A:124:ALA:HA	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:60:SER:O	1:D:64:ILE:HG13	2.02	0.60
1:B:17:PRO:HG3	1:B:45:SER:O	2.02	0.59
1:B:146:THR:HB	1:B:402:LEU:HG	1.83	0.59
1:C:123:TRP:CD2	1:C:124:ALA:HA	2.37	0.59
1:E:155:SER:HA	1:E:364:ASN:HD21	1.67	0.59
1:C:363:GLY:O	1:C:367:ARG:HD2	2.02	0.59
1:E:104:MET:HB2	1:E:105:PRO:HD3	1.84	0.59
1:C:146:THR:HB	1:C:402:LEU:HG	1.84	0.59
1:A:237:ILE:O	1:A:256:LYS:NZ	2.30	0.59
1:C:33:ILE:HG23	1:C:34:LYS:HG3	1.85	0.59
1:C:227:SER:HB2	1:C:269:LEU:HD12	1.83	0.59
1:E:196:TYR:CE1	1:E:197:ILE:HG22	2.38	0.59
1:F:110:SER:HB2	1:F:116:LEU:HD22	1.84	0.59
1:D:213:HIS:O	1:D:217:ILE:HG12	2.03	0.59
1:A:227:SER:HB2	1:A:269:LEU:HD12	1.84	0.59
1:D:227:SER:HB2	1:D:269:LEU:HD12	1.83	0.59
1:E:320:TYR:O	1:E:321:TYR:HB3	2.01	0.59
1:A:123:TRP:CZ2	1:A:408:LEU:HD13	2.37	0.59
1:B:237:ILE:O	1:B:256:LYS:NZ	2.30	0.59
1:C:290:LYS:HG3	1:C:306:GLU:HB3	1.85	0.59
1:A:421:MET:CE	1:A:425:LEU:HD21	2.33	0.59
1:E:91:VAL:HG22	1:E:120:PHE:HB3	1.85	0.59
1:E:311:PHE:HB3	1:E:314:ILE:HG13	1.84	0.59
1:E:363:GLY:O	1:E:367:ARG:HD2	2.02	0.59
1:A:178:ILE:HD11	1:A:218:LEU:HD22	1.84	0.58
1:D:146:THR:HB	1:D:402:LEU:HG	1.82	0.58
1:E:110:SER:HB2	1:E:116:LEU:HD22	1.84	0.58
1:F:363:GLY:O	1:F:367:ARG:HD2	2.03	0.58
1:C:213:HIS:O	1:C:217:ILE:HG12	2.03	0.58
1:D:33:ILE:HG23	1:D:34:LYS:HG3	1.84	0.58
1:E:156:PRO:HG3	1:E:367:ARG:NH1	2.18	0.58
1:E:227:SER:HB2	1:E:269:LEU:HD12	1.85	0.58
1:A:19:ARG:HG3	1:A:88:ASP:OD2	2.03	0.58
1:B:213:HIS:O	1:B:217:ILE:HG12	2.04	0.58
1:F:146:THR:OG1	1:F:401:THR:HB	2.03	0.58
1:A:213:HIS:O	1:A:217:ILE:HG12	2.04	0.58
1:D:290:LYS:HG3	1:D:306:GLU:HB3	1.84	0.58
1:F:104:MET:HB2	1:F:105:PRO:HD3	1.85	0.58
1:E:27:ALA:HB2	1:E:63:THR:HG23	1.86	0.58
1:A:286:LYS:HD3	1:B:297:HIS:CE1	2.38	0.58
1:F:26:ASN:O	1:F:33:ILE:HB	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:27:ALA:HB2	1:F:63:THR:HG23	1.86	0.58
1:F:18:ILE:HD12	1:F:47:PHE:CE2	2.39	0.57
1:F:91:VAL:HG22	1:F:120:PHE:HB3	1.86	0.57
1:D:410:ARG:HH22	1:D:433:TYR:HD1	1.53	0.57
1:E:35:THR:HA	1:E:362:VAL:HG22	1.86	0.57
1:E:262:LEU:HD12	1:E:262:LEU:C	2.29	0.57
1:B:427:VAL:O	1:B:427:VAL:HG13	2.02	0.57
1:D:347:LYS:N	1:D:348:GLU:CB	2.64	0.57
1:E:121:VAL:O	1:E:148:ILE:HD12	2.04	0.57
1:F:320:TYR:O	1:F:321:TYR:HB3	2.03	0.57
1:A:33:ILE:HG23	1:A:34:LYS:HG3	1.85	0.57
1:F:153:ARG:HG2	1:F:220:TYR:CG	2.39	0.57
1:B:123:TRP:CZ2	1:B:408:LEU:HD13	2.40	0.57
1:B:283:LYS:HA	1:B:284:PRO:C	2.28	0.57
1:B:123:TRP:CD2	1:B:124:ALA:HA	2.39	0.57
1:E:314:ILE:HD12	1:E:314:ILE:O	2.04	0.57
1:F:262:LEU:HD12	1:F:262:LEU:C	2.28	0.57
1:C:27:ALA:CB	1:C:67:LEU:HD21	2.35	0.57
1:C:256:LYS:HE3	1:C:260:ASP:HB3	1.87	0.57
1:F:285:THR:HB	1:F:291:ASN:HD21	1.68	0.57
1:C:123:TRP:CZ2	1:C:408:LEU:HD13	2.39	0.57
1:E:145:GLN:NE2	1:E:389:PHE:H	2.03	0.57
1:B:421:MET:CE	1:B:425:LEU:HD21	2.35	0.56
1:A:427:VAL:O	1:A:427:VAL:HG13	2.04	0.56
1:C:297:HIS:CE1	1:D:286:LYS:HD3	2.40	0.56
1:E:147:ILE:HD13	1:E:372:ILE:HD13	1.86	0.56
1:E:411:LEU:O	1:E:415:VAL:HG23	2.05	0.56
1:E:423:SER:HA	1:F:423:SER:HA	1.86	0.56
1:C:188:GLU:HB3	1:C:243:ILE:HG12	1.87	0.56
1:D:18:ILE:HD11	1:D:376:HIS:CG	2.40	0.56
1:E:153:ARG:O	1:E:154:LYS:HD3	2.05	0.56
1:D:421:MET:CE	1:D:425:LEU:HD21	2.35	0.56
1:E:256:LYS:HE2	1:E:258:VAL:O	2.05	0.56
1:E:377:PHE:O	1:E:379:THR:N	2.39	0.56
1:C:421:MET:CE	1:C:425:LEU:HD21	2.35	0.56
1:D:18:ILE:HD11	1:D:376:HIS:CD2	2.41	0.56
1:E:262:LEU:HD12	1:E:263:LEU:O	2.05	0.56
1:F:121:VAL:O	1:F:148:ILE:HD12	2.06	0.56
1:F:176:ILE:HB	1:F:275:VAL:HG22	1.87	0.56
1:A:37:TYR:HB3	1:A:38:PRO:HD3	1.88	0.56
1:C:60:SER:O	1:C:64:ILE:HG13	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:145:GLN:NE2	1:D:388:GLN:HG3	2.20	0.56
1:E:309:ALA:O	1:E:311:PHE:N	2.39	0.56
1:D:317:LEU:O	1:D:354:HIS:HD2	1.89	0.56
1:E:191:VAL:HG23	1:E:243:ILE:O	2.06	0.56
1:B:363:GLY:O	1:B:367:ARG:HD2	2.06	0.56
1:A:297:HIS:NE2	1:B:286:LYS:HD3	2.21	0.55
1:B:33:ILE:HG23	1:B:34:LYS:HG3	1.88	0.55
1:E:96:VAL:HA	1:E:99:HIS:CD2	2.41	0.55
1:E:285:THR:HB	1:E:291:ASN:HD21	1.70	0.55
1:E:304:LYS:HG2	1:E:305:LEU:N	2.16	0.55
1:A:60:SER:O	1:A:64:ILE:HG13	2.05	0.55
1:D:27:ALA:CB	1:D:67:LEU:HD21	2.36	0.55
1:F:227:SER:HB2	1:F:269:LEU:HD12	1.89	0.55
1:A:324:THR:O	1:A:325:ARG:C	2.50	0.55
1:B:60:SER:O	1:B:64:ILE:HG13	2.07	0.55
1:D:37:TYR:HB3	1:D:38:PRO:HD3	1.88	0.55
1:F:122:GLU:HA	1:F:149:SER:HB3	1.88	0.55
1:E:290:LYS:HG3	1:E:306:GLU:HB3	1.88	0.55
1:B:64:ILE:HG23	1:B:72:ALA:HB3	1.88	0.55
1:E:146:THR:OG1	1:E:401:THR:HB	2.07	0.55
1:F:410:ARG:HB3	1:F:430:ILE:HD12	1.89	0.55
1:D:155:SER:HB3	1:D:158:ILE:HD13	1.88	0.54
1:E:413:GLU:O	1:E:417:LYS:HB2	2.07	0.54
1:F:96:VAL:HA	1:F:99:HIS:CD2	2.42	0.54
1:D:283:LYS:HA	1:D:284:PRO:C	2.32	0.54
1:E:297:HIS:CE1	1:F:286:LYS:HG2	2.42	0.54
1:D:323:GLY:O	1:D:324:THR:C	2.50	0.54
1:B:375:PHE:CZ	1:B:387:SER:O	2.60	0.54
1:E:65:GLN:O	1:E:66:ARG:C	2.51	0.54
1:E:322:SER:OG	1:E:323:GLY:N	2.41	0.54
1:A:420:MET:HE2	1:A:420:MET:HA	1.90	0.54
1:F:236:ASN:O	1:F:238:PRO:HD3	2.07	0.54
1:A:258:VAL:HG22	1:A:259:PRO:CD	2.38	0.54
1:A:256:LYS:HD2	1:A:258:VAL:HG12	1.89	0.54
1:B:256:LYS:HG2	1:B:258:VAL:H	1.73	0.54
1:B:375:PHE:HZ	1:B:387:SER:O	1.91	0.53
1:D:256:LYS:HD2	1:D:258:VAL:HG12	1.90	0.53
1:E:153:ARG:HD2	1:E:400:PRO:HG3	1.90	0.53
1:E:264:PHE:O	1:E:265:GLN:HB2	2.06	0.53
1:B:256:LYS:HE3	1:B:260:ASP:HB3	1.90	0.53
1:B:420:MET:HA	1:B:420:MET:HE2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:TYR:HB3	1:C:38:PRO:HD3	1.91	0.53
1:D:188:GLU:HB3	1:D:243:ILE:HG12	1.90	0.53
1:B:120:PHE:HD2	1:B:121:VAL:N	2.07	0.53
1:E:106:LEU:C	1:E:106:LEU:HD23	2.32	0.53
1:B:256:LYS:HD2	1:B:258:VAL:HG12	1.90	0.53
1:C:420:MET:HE2	1:C:420:MET:HA	1.91	0.53
1:E:96:VAL:HG13	1:E:124:ALA:O	2.08	0.53
1:F:96:VAL:HG13	1:F:124:ALA:O	2.08	0.53
1:C:155:SER:HB3	1:C:158:ILE:HD13	1.90	0.53
1:F:82:ALA:HB2	1:F:106:LEU:HG	1.91	0.53
1:A:433:TYR:C	1:A:435:LEU:H	2.17	0.53
1:C:57:ILE:HD12	1:C:76:PRO:CA	2.36	0.53
1:F:264:PHE:CG	1:F:265:GLN:N	2.77	0.53
1:E:190:PRO:HA	1:E:243:ILE:HD12	1.90	0.53
1:F:361:ILE:H	1:F:361:ILE:CD1	2.20	0.53
1:A:64:ILE:HG23	1:A:72:ALA:HB3	1.91	0.53
1:A:317:LEU:O	1:A:354:HIS:HD2	1.92	0.53
1:A:387:SER:O	1:A:388:GLN:C	2.51	0.53
1:E:123:TRP:CH2	1:E:408:LEU:HD13	2.43	0.53
1:C:287:LYS:HE3	1:D:348:GLU:OE1	2.09	0.53
1:D:427:VAL:O	1:D:427:VAL:CG1	2.57	0.53
1:E:427:VAL:HG12	1:E:430:ILE:HG12	1.88	0.53
1:F:65:GLN:O	1:F:66:ARG:C	2.51	0.53
1:A:283:LYS:HA	1:A:284:PRO:C	2.34	0.52
1:C:283:LYS:HA	1:C:284:PRO:C	2.34	0.52
1:E:122:GLU:HA	1:E:149:SER:HB3	1.90	0.52
1:A:57:ILE:HD12	1:A:76:PRO:CA	2.37	0.52
1:F:264:PHE:O	1:F:265:GLN:HB2	2.08	0.52
1:C:427:VAL:O	1:C:427:VAL:HG13	2.09	0.52
1:A:242:LEU:HD12	1:A:252:GLN:HG2	1.92	0.52
1:A:188:GLU:HB3	1:A:243:ILE:HG12	1.92	0.52
1:B:106:LEU:HD23	1:B:106:LEU:C	2.34	0.52
1:B:155:SER:HB3	1:B:158:ILE:HD13	1.91	0.52
1:D:361:ILE:HD12	1:D:361:ILE:H	1.75	0.52
1:E:92:ILE:HB	1:E:121:VAL:HG22	1.92	0.52
1:D:432:HIS:O	1:D:433:TYR:HB2	2.09	0.52
1:F:106:LEU:C	1:F:106:LEU:HD23	2.34	0.52
1:B:37:TYR:HB3	1:B:38:PRO:HD3	1.92	0.51
1:D:120:PHE:HD2	1:D:121:VAL:N	2.07	0.51
1:F:123:TRP:CH2	1:F:408:LEU:HD13	2.44	0.51
1:D:258:VAL:HG22	1:D:259:PRO:CD	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:161:ALA:O	1:F:165:ILE:HG13	2.10	0.51
1:A:256:LYS:HE3	1:A:260:ASP:HB3	1.92	0.51
1:A:434:SER:O	1:A:435:LEU:C	2.53	0.51
1:B:188:GLU:HB3	1:B:243:ILE:HG12	1.92	0.51
1:C:256:LYS:HG2	1:C:258:VAL:H	1.75	0.51
1:C:387:SER:O	1:C:388:GLN:C	2.53	0.51
1:D:420:MET:HA	1:D:420:MET:HE2	1.92	0.51
1:E:82:ALA:HB2	1:E:106:LEU:HG	1.93	0.51
1:E:169:TYR:CE2	1:E:323:GLY:HA3	2.46	0.51
1:A:426:ASN:HB3	1:C:423:SER:CB	2.40	0.51
1:C:64:ILE:HG23	1:C:72:ALA:HB3	1.92	0.51
1:C:286:LYS:HD3	1:D:297:HIS:CE1	2.46	0.51
1:D:256:LYS:HG2	1:D:258:VAL:H	1.75	0.51
1:E:350:MET:O	1:E:351:LYS:HG3	2.10	0.51
1:F:155:SER:HB3	1:F:158:ILE:HB	1.92	0.51
1:B:27:ALA:CB	1:B:67:LEU:HD21	2.37	0.51
1:D:57:ILE:HD12	1:D:76:PRO:CA	2.38	0.51
1:D:106:LEU:C	1:D:106:LEU:HD23	2.36	0.51
1:A:120:PHE:HD2	1:A:121:VAL:N	2.09	0.51
1:C:317:LEU:O	1:C:354:HIS:HD2	1.93	0.51
1:E:361:ILE:HD12	1:E:361:ILE:H	1.76	0.51
1:F:427:VAL:O	1:F:427:VAL:CG1	2.58	0.51
1:A:256:LYS:HG2	1:A:258:VAL:H	1.75	0.51
1:C:120:PHE:HD2	1:C:121:VAL:N	2.09	0.51
1:E:54:SER:HB3	1:E:55:PRO:HD2	1.93	0.51
1:E:236:ASN:O	1:E:238:PRO:HD3	2.10	0.51
1:F:153:ARG:HG2	1:F:220:TYR:CD1	2.45	0.51
1:F:427:VAL:O	1:F:427:VAL:HG12	2.10	0.51
1:A:16:ALA:N	1:A:17:PRO:HD3	2.26	0.51
1:D:35:THR:HB	1:D:365:ILE:HG13	1.93	0.51
1:E:123:TRP:CZ2	1:E:408:LEU:HD13	2.46	0.51
1:E:408:LEU:HD22	1:E:412:ILE:HD11	1.92	0.51
1:E:264:PHE:CG	1:E:265:GLN:N	2.78	0.50
1:F:303:LEU:HD23	1:F:304:LYS:N	2.25	0.50
1:E:258:VAL:HG13	1:E:259:PRO:CD	2.40	0.50
1:C:256:LYS:HD2	1:C:258:VAL:HG12	1.93	0.50
1:D:123:TRP:CZ2	1:D:408:LEU:HD13	2.46	0.50
1:B:361:ILE:HD12	1:B:361:ILE:H	1.77	0.50
1:E:169:TYR:HE2	1:E:322:SER:O	1.94	0.50
1:B:18:ILE:HD11	1:B:376:HIS:CG	2.46	0.50
1:A:155:SER:HB3	1:A:158:ILE:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:LYS:HZ3	1:C:417:LYS:HG3	1.76	0.50
1:B:35:THR:HB	1:B:365:ILE:HG13	1.94	0.50
1:D:256:LYS:HE3	1:D:260:ASP:HB3	1.92	0.50
1:B:258:VAL:HG22	1:B:259:PRO:CD	2.42	0.50
1:E:413:GLU:HA	1:E:413:GLU:OE1	2.11	0.50
1:A:27:ALA:CB	1:A:67:LEU:HD21	2.37	0.50
1:B:178:ILE:CD1	1:B:218:LEU:HD22	2.41	0.50
1:B:242:LEU:HD12	1:B:252:GLN:HG2	1.94	0.50
1:E:320:TYR:HB3	1:F:288:PHE:CD2	2.47	0.50
1:D:64:ILE:HG23	1:D:72:ALA:HB3	1.93	0.49
1:F:102:VAL:O	1:F:105:PRO:HD2	2.11	0.49
1:F:349:ILE:HG22	1:F:350:MET:N	2.25	0.49
1:A:35:THR:HB	1:A:365:ILE:HG13	1.93	0.49
1:C:106:LEU:C	1:C:106:LEU:HD23	2.37	0.49
1:F:236:ASN:C	1:F:238:PRO:HD3	2.36	0.49
1:A:79:GLU:HG3	1:A:109:PHE:CD2	2.46	0.49
1:A:417:LYS:CG	1:C:417:LYS:HZ3	2.20	0.49
1:E:102:VAL:O	1:E:105:PRO:HD2	2.12	0.49
1:F:145:GLN:HE22	1:F:389:PHE:H	1.60	0.49
1:A:106:LEU:C	1:A:106:LEU:HD23	2.38	0.49
1:F:322:SER:CB	1:F:350:MET:HG2	2.43	0.49
1:F:390:VAL:HG13	1:F:391:MET:HG2	1.94	0.49
1:B:427:VAL:O	1:B:427:VAL:CG1	2.60	0.49
1:E:236:ASN:C	1:E:238:PRO:HD3	2.37	0.49
1:F:21:GLY:H	1:F:87:ILE:HG23	1.78	0.49
1:B:317:LEU:O	1:B:354:HIS:HD2	1.95	0.49
1:F:54:SER:HB3	1:F:55:PRO:HD2	1.93	0.49
1:F:123:TRP:CZ2	1:F:408:LEU:HD13	2.47	0.49
1:C:35:THR:HB	1:C:365:ILE:HG13	1.95	0.49
1:C:408:LEU:O	1:C:412:ILE:HG12	2.13	0.49
1:E:182:GLY:O	1:E:184:TRP:N	2.39	0.49
1:B:57:ILE:HD12	1:B:76:PRO:CA	2.42	0.49
1:C:258:VAL:HG22	1:C:259:PRO:CD	2.42	0.49
1:A:158:ILE:HG12	1:A:217:ILE:CG2	2.41	0.49
1:F:351:LYS:O	1:F:352:VAL:HG23	2.12	0.49
1:A:197:ILE:HG12	1:A:198:TYR:CE1	2.48	0.48
1:C:207:VAL:O	1:C:211:PHE:HB3	2.13	0.48
1:F:60:SER:HB3	1:F:74:ALA:HB1	1.95	0.48
1:F:155:SER:HB3	1:F:158:ILE:HD13	1.94	0.48
1:A:427:VAL:O	1:A:427:VAL:CG1	2.62	0.48
1:F:258:VAL:HG13	1:F:259:PRO:CD	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:VAL:HG22	1:A:259:PRO:HD3	1.95	0.48
1:B:145:GLN:HE21	1:B:388:GLN:HG3	1.78	0.48
1:C:158:ILE:HG12	1:C:217:ILE:CG2	2.43	0.48
1:A:123:TRP:CH2	1:A:408:LEU:HD13	2.49	0.48
1:A:322:SER:HB3	1:A:350:MET:HG2	1.96	0.48
1:C:242:LEU:HD12	1:C:252:GLN:HG2	1.95	0.48
1:C:322:SER:OG	1:D:287:LYS:HG3	2.13	0.48
1:F:262:LEU:HD12	1:F:263:LEU:C	2.38	0.48
1:E:295:ASP:OD1	1:E:304:LYS:HE2	2.14	0.48
1:E:354:HIS:CD2	1:E:355:LEU:N	2.82	0.48
1:F:302:ASP:O	1:F:303:LEU:HB2	2.14	0.48
1:B:408:LEU:O	1:B:412:ILE:HG12	2.13	0.48
1:C:123:TRP:CH2	1:C:408:LEU:HD13	2.48	0.48
1:C:361:ILE:H	1:C:361:ILE:HD12	1.79	0.48
1:D:158:ILE:HG12	1:D:217:ILE:CG2	2.43	0.48
1:E:123:TRP:CD2	1:E:124:ALA:N	2.65	0.48
1:D:258:VAL:HG22	1:D:259:PRO:HD3	1.96	0.48
1:E:352:VAL:CG1	1:E:353:TYR:N	2.76	0.48
1:F:179:ALA:HB1	1:F:286:LYS:NZ	2.29	0.48
1:F:363:GLY:O	1:F:366:HIS:HB3	2.14	0.48
1:B:197:ILE:HG12	1:B:198:TYR:CE1	2.49	0.47
1:D:242:LEU:HD12	1:D:252:GLN:HG2	1.96	0.47
1:E:286:LYS:HG2	1:F:297:HIS:CE1	2.49	0.47
1:F:147:ILE:HD13	1:F:372:ILE:HD13	1.96	0.47
1:B:231:ALA:CB	1:B:415:VAL:HG13	2.44	0.47
1:F:349:ILE:HD12	1:F:349:ILE:H	1.79	0.47
1:A:146:THR:C	1:A:147:ILE:HG13	2.40	0.47
1:D:76:PRO:HD2	1:D:80:SER:OG	2.15	0.47
1:E:243:ILE:O	1:E:243:ILE:HD12	2.14	0.47
1:F:397:GLU:CD	1:F:397:GLU:H	2.21	0.47
1:E:353:TYR:C	1:E:353:TYR:CD2	2.92	0.47
1:F:314:ILE:HD12	1:F:314:ILE:O	2.14	0.47
1:F:361:ILE:HD12	1:F:361:ILE:N	2.22	0.47
1:A:417:LYS:NZ	1:C:417:LYS:HG3	2.29	0.47
1:B:217:ILE:HG12	1:B:217:ILE:H	1.45	0.47
1:B:417:LYS:O	1:B:421:MET:HG3	2.15	0.47
1:E:174:ASN:ND2	1:F:187:TYR:CE1	2.83	0.47
1:A:423:SER:CB	1:C:426:ASN:HB3	2.45	0.47
1:C:79:GLU:HG3	1:C:109:PHE:CD2	2.50	0.47
1:C:181:ASN:OD1	1:C:282:GLY:HA2	2.15	0.47
1:E:367:ARG:O	1:E:370:GLN:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:397:GLU:H	1:E:397:GLU:CD	2.22	0.47
1:F:181:ASN:ND2	1:F:280:LYS:HB3	2.29	0.47
1:F:349:ILE:CG2	1:F:350:MET:N	2.77	0.47
1:C:314:ILE:HD12	1:C:314:ILE:O	2.15	0.47
1:A:265:GLN:NE2	1:B:265:GLN:HB2	2.30	0.47
1:C:145:GLN:NE2	1:C:388:GLN:HG3	2.29	0.47
1:E:174:ASN:HD22	1:F:187:TYR:HE1	1.62	0.47
1:E:376:HIS:CD2	1:E:377:PHE:CE1	2.96	0.47
1:F:147:ILE:HG21	1:F:372:ILE:HD11	1.97	0.47
1:F:237:ILE:O	1:F:256:LYS:NZ	2.48	0.47
1:A:286:LYS:HD3	1:B:297:HIS:NE2	2.30	0.46
1:A:361:ILE:HD12	1:A:361:ILE:H	1.79	0.46
1:B:145:GLN:NE2	1:B:388:GLN:HG3	2.30	0.46
1:E:349:ILE:N	1:E:349:ILE:HD12	2.30	0.46
1:F:181:ASN:OD1	1:F:282:GLY:HA2	2.15	0.46
1:A:283:LYS:HB3	1:A:284:PRO:HA	1.97	0.46
1:F:23:VAL:HG23	1:F:81:PHE:CZ	2.51	0.46
1:F:303:LEU:HD23	1:F:303:LEU:C	2.41	0.46
1:D:256:LYS:HE2	1:D:258:VAL:O	2.15	0.46
1:E:363:GLY:O	1:E:366:HIS:HB3	2.15	0.46
1:F:153:ARG:HD3	1:F:392:GLN:OE1	2.14	0.46
1:F:200:ILE:HG12	1:F:201:GLY:N	2.30	0.46
1:B:158:ILE:HG12	1:B:217:ILE:CG2	2.44	0.46
1:E:303:LEU:HD23	1:E:303:LEU:C	2.41	0.46
1:E:181:ASN:OD1	1:E:282:GLY:HA2	2.16	0.46
1:F:27:ALA:CB	1:F:67:LEU:HD21	2.46	0.46
1:F:147:ILE:HD13	1:F:372:ILE:CD1	2.45	0.46
1:B:349:ILE:O	1:B:349:ILE:HG22	2.15	0.46
1:D:108:GLU:HA	1:D:108:GLU:OE2	2.14	0.46
1:E:21:GLY:H	1:E:87:ILE:HG23	1.80	0.46
1:F:122:GLU:HA	1:F:149:SER:CB	2.45	0.46
1:C:231:ALA:CB	1:C:415:VAL:HG13	2.46	0.46
1:E:27:ALA:CB	1:E:67:LEU:HD21	2.46	0.46
1:F:306:GLU:O	1:F:317:LEU:HD22	2.16	0.46
1:A:430:ILE:HD13	1:A:430:ILE:HA	1.66	0.46
1:E:122:GLU:HA	1:E:149:SER:CB	2.46	0.46
1:E:200:ILE:HG12	1:E:201:GLY:N	2.31	0.46
1:A:108:GLU:OE2	1:A:108:GLU:HA	2.16	0.46
1:C:256:LYS:HE2	1:C:258:VAL:O	2.16	0.46
1:E:237:ILE:O	1:E:256:LYS:NZ	2.49	0.46
1:F:92:ILE:HB	1:F:121:VAL:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:ILE:HG12	1:A:198:TYR:CD1	2.51	0.45
1:B:207:VAL:O	1:B:211:PHE:HB3	2.14	0.45
1:F:264:PHE:CD2	1:F:265:GLN:N	2.84	0.45
1:F:320:TYR:CD2	1:F:352:VAL:HG22	2.51	0.45
1:A:147:ILE:HG12	1:A:399:PHE:CE2	2.51	0.45
1:B:79:GLU:HG3	1:B:109:PHE:CD2	2.51	0.45
1:F:147:ILE:HG12	1:F:399:PHE:CE2	2.51	0.45
1:A:313:GLU:HG2	1:A:314:ILE:HG23	1.99	0.45
1:A:408:LEU:O	1:A:412:ILE:HG12	2.17	0.45
1:B:76:PRO:HD2	1:B:80:SER:OG	2.17	0.45
1:E:232:MET:HB2	1:E:263:LEU:HB2	1.98	0.45
1:E:262:LEU:HD12	1:E:263:LEU:C	2.42	0.45
1:F:96:VAL:HG11	1:F:124:ALA:HB1	1.98	0.45
1:F:178:ILE:HB	1:F:277:CYS:SG	2.57	0.45
1:C:197:ILE:O	1:C:197:ILE:HG13	2.16	0.45
1:D:181:ASN:OD1	1:D:282:GLY:HA2	2.16	0.45
1:D:408:LEU:O	1:D:412:ILE:HG12	2.15	0.45
1:E:60:SER:HB3	1:E:74:ALA:HB1	1.97	0.45
1:B:256:LYS:HE2	1:B:258:VAL:O	2.16	0.45
1:C:178:ILE:CD1	1:C:218:LEU:HD22	2.45	0.45
1:D:58:GLU:H	1:D:58:GLU:HG3	1.48	0.45
1:D:313:GLU:HG2	1:D:314:ILE:HG23	1.98	0.45
1:E:104:MET:HE1	1:E:138:ALA:HB2	1.99	0.45
1:B:123:TRP:CH2	1:B:408:LEU:HD13	2.51	0.45
1:B:197:ILE:HG12	1:B:198:TYR:CD1	2.51	0.45
1:B:197:ILE:O	1:B:197:ILE:HG13	2.17	0.45
1:C:58:GLU:H	1:C:58:GLU:HG3	1.51	0.45
1:D:83:SER:OG	1:D:112:ASN:HB2	2.16	0.45
1:D:207:VAL:O	1:D:211:PHE:HB3	2.16	0.45
1:D:376:HIS:C	1:D:378:ASN:H	2.24	0.45
1:E:163:GLU:O	1:E:167:GLN:HG3	2.16	0.45
1:B:432:HIS:O	1:B:433:TYR:C	2.60	0.45
1:B:145:GLN:HE22	1:B:389:PHE:H	1.64	0.45
1:C:83:SER:OG	1:C:112:ASN:HB2	2.17	0.45
1:F:41:LEU:C	1:F:43:LEU:H	2.24	0.45
1:A:83:SER:OG	1:A:112:ASN:HB2	2.17	0.45
1:D:197:ILE:HG12	1:D:198:TYR:CE1	2.51	0.45
1:E:311:PHE:HD1	1:E:313:GLU:OE2	2.00	0.45
1:B:181:ASN:OD1	1:B:282:GLY:HA2	2.16	0.45
1:D:283:LYS:HB3	1:D:284:PRO:HA	1.97	0.45
1:E:192:LYS:O	1:E:193:SER:C	2.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:157:TYR:CD1	1:F:157:TYR:N	2.80	0.45
1:F:60:SER:HB3	1:F:74:ALA:CB	2.46	0.44
1:B:83:SER:OG	1:B:112:ASN:HB2	2.17	0.44
1:E:147:ILE:HG21	1:E:372:ILE:HD11	1.99	0.44
1:A:322:SER:OG	1:B:287:LYS:HG3	2.18	0.44
1:C:108:GLU:OE2	1:C:108:GLU:HA	2.16	0.44
1:C:432:HIS:O	1:C:433:TYR:O	2.35	0.44
1:F:89:MET:HE1	1:F:372:ILE:HG21	1.98	0.44
1:F:170:ILE:HB	1:F:301:GLY:O	2.17	0.44
1:D:197:ILE:HG12	1:D:198:TYR:CD1	2.52	0.44
1:F:411:LEU:O	1:F:415:VAL:HG23	2.17	0.44
1:A:417:LYS:O	1:A:421:MET:HG3	2.17	0.44
1:B:108:GLU:HA	1:B:108:GLU:OE2	2.17	0.44
1:F:190:PRO:HA	1:F:243:ILE:HD12	1.99	0.44
1:A:89:MET:HB2	1:A:118:TYR:HB2	2.00	0.44
1:A:197:ILE:O	1:A:197:ILE:HG13	2.18	0.44
1:B:193:SER:HA	1:B:194:PRO:HD3	1.75	0.44
1:C:76:PRO:HD2	1:C:80:SER:OG	2.18	0.44
1:E:23:VAL:HG23	1:E:81:PHE:CZ	2.51	0.44
1:B:120:PHE:C	1:B:120:PHE:CD2	2.96	0.44
1:B:258:VAL:HG22	1:B:259:PRO:HD3	1.99	0.44
1:C:110:SER:HB2	1:C:116:LEU:HD22	1.99	0.44
1:E:156:PRO:HG3	1:E:367:ARG:CZ	2.48	0.44
1:F:262:LEU:O	1:F:262:LEU:HG	2.17	0.44
1:B:110:SER:HB2	1:B:116:LEU:HD22	1.99	0.44
1:C:376:HIS:HD2	1:C:377:PHE:CD1	2.36	0.44
1:C:427:VAL:O	1:C:427:VAL:CG1	2.65	0.44
1:E:41:LEU:C	1:E:43:LEU:H	2.25	0.44
1:E:129:LEU:HD12	1:E:413:GLU:HG2	1.99	0.44
1:F:241:GLU:HG2	1:F:249:ARG:HD3	1.98	0.44
1:B:147:ILE:HG12	1:B:399:PHE:CE2	2.52	0.44
1:D:231:ALA:CB	1:D:415:VAL:HG13	2.48	0.44
1:A:178:ILE:HB	1:A:277:CYS:SG	2.58	0.43
1:B:243:ILE:CG2	1:B:249:ARG:HG2	2.48	0.43
1:E:249:ARG:C	1:E:251:GLY:H	2.26	0.43
1:F:37:TYR:C	1:F:39:ALA:H	2.26	0.43
1:A:265:GLN:HB2	1:B:265:GLN:NE2	2.34	0.43
1:B:283:LYS:HB3	1:B:284:PRO:HA	2.00	0.43
1:B:430:ILE:HD13	1:B:430:ILE:HA	1.66	0.43
1:C:197:ILE:HG12	1:C:198:TYR:CE1	2.53	0.43
1:E:178:ILE:HD11	1:E:218:LEU:HD13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:160:ARG:NH1	1:F:353:TYR:CE1	2.86	0.43
1:A:347:LYS:HD3	1:A:347:LYS:C	2.43	0.43
1:B:58:GLU:H	1:B:58:GLU:HG3	1.48	0.43
1:B:245:GLU:OE1	1:B:245:GLU:HA	2.18	0.43
1:E:147:ILE:HG12	1:E:399:PHE:CE2	2.53	0.43
1:F:50:THR:HG21	1:F:86:THR:O	2.18	0.43
1:F:123:TRP:HE1	1:F:209:THR:HA	1.84	0.43
1:F:249:ARG:C	1:F:251:GLY:H	2.27	0.43
1:A:76:PRO:HD2	1:A:80:SER:OG	2.19	0.43
1:A:155:SER:HA	1:A:364:ASN:ND2	2.33	0.43
1:E:115:ASN:HD22	1:E:115:ASN:HA	1.52	0.43
1:C:146:THR:C	1:C:147:ILE:HG13	2.43	0.43
1:C:217:ILE:HG12	1:C:217:ILE:H	1.46	0.43
1:C:417:LYS:O	1:C:421:MET:HG3	2.17	0.43
1:D:120:PHE:C	1:D:120:PHE:CD2	2.96	0.43
1:E:60:SER:HB3	1:E:74:ALA:CB	2.48	0.43
1:F:243:ILE:HD12	1:F:243:ILE:O	2.18	0.43
1:A:110:SER:HB2	1:A:116:LEU:HD22	1.99	0.43
1:B:145:GLN:NE2	1:B:389:PHE:H	2.17	0.43
1:B:146:THR:C	1:B:147:ILE:HG13	2.43	0.43
1:C:430:ILE:HD13	1:C:430:ILE:HA	1.64	0.43
1:D:178:ILE:CD1	1:D:218:LEU:HD22	2.47	0.43
1:F:314:ILE:HB	1:F:361:ILE:HG13	2.00	0.43
1:D:79:GLU:HG3	1:D:109:PHE:CD2	2.54	0.43
1:D:243:ILE:CG2	1:D:249:ARG:HG2	2.49	0.43
1:E:96:VAL:HG11	1:E:124:ALA:HB1	1.99	0.43
1:F:104:MET:HE1	1:F:138:ALA:HB2	2.00	0.43
1:F:356:ARG:O	1:F:357:ASN:HB2	2.19	0.43
1:A:221:MET:HE1	1:A:294:ILE:HG21	2.01	0.43
1:B:89:MET:HB2	1:B:118:TYR:HB2	2.00	0.43
1:B:178:ILE:HB	1:B:277:CYS:SG	2.59	0.43
1:D:214:THR:O	1:D:217:ILE:HG13	2.19	0.43
1:E:241:GLU:HG2	1:E:249:ARG:HD3	2.01	0.43
1:F:323:GLY:O	1:F:324:THR:C	2.62	0.43
1:A:178:ILE:CD1	1:A:218:LEU:HD22	2.47	0.43
1:E:21:GLY:N	1:E:87:ILE:HG23	2.34	0.43
1:E:169:TYR:CE2	1:E:322:SER:O	2.71	0.43
1:F:232:MET:HB2	1:F:263:LEU:HB2	2.00	0.43
1:C:190:PRO:HA	1:C:243:ILE:O	2.19	0.42
1:C:197:ILE:HG12	1:C:198:TYR:CD1	2.54	0.42
1:D:430:ILE:HD13	1:D:430:ILE:HA	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:262:LEU:HD11	1:F:264:PHE:HB2	2.00	0.42
1:A:207:VAL:O	1:A:211:PHE:HB3	2.19	0.42
1:C:120:PHE:C	1:C:120:PHE:CD2	2.97	0.42
1:D:147:ILE:HG12	1:D:399:PHE:CE2	2.54	0.42
1:E:75:PHE:HA	1:E:76:PRO:HD3	1.71	0.42
1:F:153:ARG:O	1:F:154:LYS:HD3	2.18	0.42
1:A:245:GLU:HA	1:A:245:GLU:OE1	2.18	0.42
1:C:75:PHE:HA	1:C:76:PRO:HD3	1.72	0.42
1:A:120:PHE:C	1:A:120:PHE:CD2	2.97	0.42
1:C:16:ALA:N	1:C:17:PRO:HD3	2.34	0.42
1:E:174:ASN:ND2	1:F:187:TYR:HE1	2.15	0.42
1:C:243:ILE:CG2	1:C:249:ARG:HG2	2.49	0.42
1:C:245:GLU:OE1	1:C:245:GLU:HA	2.18	0.42
1:C:285:THR:HB	1:C:291:ASN:ND2	2.29	0.42
1:D:347:LYS:HE2	1:D:347:LYS:HB2	1.92	0.42
1:F:160:ARG:NH1	1:F:353:TYR:HE1	2.17	0.42
1:A:314:ILE:HD12	1:A:314:ILE:O	2.19	0.42
1:B:376:HIS:C	1:B:378:ASN:H	2.28	0.42
1:D:151:GLN:O	1:D:152:GLY:C	2.63	0.42
1:D:245:GLU:HA	1:D:245:GLU:OE1	2.19	0.42
1:E:29:LYS:HB3	1:E:30:GLY:H	1.72	0.42
1:A:151:GLN:O	1:A:152:GLY:C	2.63	0.42
1:C:89:MET:HB2	1:C:118:TYR:HB2	2.02	0.42
1:C:189:ARG:HA	1:C:190:PRO:HD3	1.92	0.42
1:C:227:SER:HB3	1:C:267:THR:OG1	2.20	0.42
1:D:325:ARG:HG3	1:D:348:GLU:HB3	2.01	0.42
1:F:180:GLY:HA3	1:F:279:PHE:CE2	2.55	0.42
1:A:181:ASN:OD1	1:A:282:GLY:HA2	2.20	0.42
1:A:243:ILE:CG2	1:A:249:ARG:HG2	2.50	0.42
1:B:107:LEU:HD13	1:B:107:LEU:HA	1.83	0.42
1:B:129:LEU:HD23	1:B:129:LEU:HA	1.83	0.42
1:E:158:ILE:N	1:E:158:ILE:HD12	2.34	0.42
1:E:265:GLN:OE1	1:F:265:GLN:OE1	2.37	0.42
1:E:318:VAL:HG22	1:E:354:HIS:CG	2.55	0.42
1:A:417:LYS:HD2	1:C:417:LYS:HD2	2.02	0.42
1:E:172:ASP:O	1:E:299:THR:HG23	2.19	0.42
1:E:264:PHE:CD2	1:E:265:GLN:N	2.88	0.42
1:E:367:ARG:O	1:E:368:LEU:C	2.63	0.42
1:F:85:SER:HA	1:F:113:ASN:OD1	2.20	0.42
1:F:115:ASN:HD22	1:F:115:ASN:HA	1.51	0.42
1:F:197:ILE:HG13	1:F:198:TYR:CD1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:297:HIS:CE1	1:D:286:LYS:HG2	2.54	0.41
1:E:207:VAL:HB	1:E:416:TYR:OH	2.20	0.41
1:F:95:GLN:HG2	1:F:196:TYR:OH	2.20	0.41
1:A:231:ALA:CB	1:A:415:VAL:HG13	2.50	0.41
1:D:197:ILE:O	1:D:197:ILE:HG13	2.19	0.41
1:E:123:TRP:HE1	1:E:209:THR:HA	1.86	0.41
1:F:214:THR:O	1:F:217:ILE:CG1	2.67	0.41
1:A:190:PRO:HA	1:A:243:ILE:O	2.20	0.41
1:C:147:ILE:HG12	1:C:399:PHE:CE2	2.55	0.41
1:C:194:PRO:HB2	1:C:196:TYR:CD2	2.55	0.41
1:D:89:MET:HB2	1:D:118:TYR:HB2	2.02	0.41
1:D:314:ILE:O	1:D:314:ILE:HD12	2.20	0.41
1:E:262:LEU:O	1:E:262:LEU:HG	2.20	0.41
1:E:284:PRO:HB3	1:F:325:ARG:HH22	1.86	0.41
1:E:288:PHE:CD2	1:F:320:TYR:HB3	2.54	0.41
1:F:302:ASP:HB3	1:F:303:LEU:H	1.65	0.41
1:B:221:MET:HE1	1:B:294:ILE:HG21	2.03	0.41
1:B:313:GLU:HG2	1:B:314:ILE:HG23	2.02	0.41
1:D:123:TRP:CD1	1:D:124:ALA:N	2.88	0.41
1:F:290:LYS:HG3	1:F:306:GLU:HB3	2.01	0.41
1:A:271:GLY:O	1:A:272:ASN:C	2.63	0.41
1:A:432:HIS:HB2	1:A:433:TYR:H	1.47	0.41
1:C:214:THR:O	1:C:217:ILE:HG13	2.20	0.41
1:C:214:THR:HA	1:C:217:ILE:HG13	2.02	0.41
1:F:169:TYR:CE2	1:F:323:GLY:HA3	2.55	0.41
1:D:67:LEU:H	1:D:67:LEU:HG	1.61	0.41
1:D:178:ILE:HB	1:D:277:CYS:SG	2.60	0.41
1:F:146:THR:C	1:F:147:ILE:HG13	2.44	0.41
1:F:355:LEU:O	1:F:356:ARG:C	2.64	0.41
1:E:389:PHE:CE1	1:E:401:THR:HG21	2.56	0.41
1:A:145:GLN:NE2	1:A:388:GLN:HG3	2.36	0.41
1:A:420:MET:SD	1:C:433:TYR:CE1	3.14	0.41
1:C:376:HIS:HD2	1:C:377:PHE:CE1	2.38	0.41
1:E:421:MET:HE3	1:E:421:MET:HB3	1.89	0.41
1:A:180:GLY:HA3	1:A:279:PHE:CE2	2.55	0.41
1:A:230:ASN:ND2	1:B:230:ASN:ND2	2.69	0.41
1:B:120:PHE:HD2	1:B:120:PHE:C	2.29	0.41
1:B:148:ILE:HG22	1:B:400:PRO:HB2	2.03	0.41
1:B:190:PRO:HA	1:B:243:ILE:O	2.20	0.41
1:C:104:MET:HE1	1:C:138:ALA:HB2	2.03	0.41
1:C:221:MET:HE1	1:C:294:ILE:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:421:MET:HE2	1:C:425:LEU:HD21	2.03	0.41
1:D:110:SER:HB2	1:D:116:LEU:HD22	2.03	0.41
1:D:214:THR:HA	1:D:217:ILE:HG13	2.03	0.41
1:E:37:TYR:C	1:E:39:ALA:H	2.27	0.41
1:F:153:ARG:CD	1:F:400:PRO:HG3	2.47	0.41
1:F:192:LYS:O	1:F:193:SER:C	2.62	0.41
1:F:388:GLN:O	1:F:389:PHE:HB3	2.20	0.41
1:F:424:THR:HG22	1:F:425:LEU:N	2.36	0.41
1:A:227:SER:HB3	1:A:267:THR:OG1	2.21	0.41
1:A:256:LYS:HE2	1:A:258:VAL:O	2.20	0.41
1:B:194:PRO:HB2	1:B:196:TYR:CD2	2.56	0.41
1:D:75:PHE:HA	1:D:76:PRO:HD3	1.77	0.41
1:E:43:LEU:HD11	1:E:366:HIS:NE2	2.36	0.41
1:E:89:MET:HB2	1:E:118:TYR:HB2	2.03	0.41
1:A:104:MET:HE1	1:A:138:ALA:HB2	2.03	0.40
1:C:35:THR:O	1:C:38:PRO:HD2	2.21	0.40
1:D:146:THR:C	1:D:147:ILE:HG13	2.46	0.40
1:D:180:GLY:HA3	1:D:279:PHE:CE2	2.56	0.40
1:D:317:LEU:O	1:D:354:HIS:CD2	2.71	0.40
1:E:389:PHE:HE1	1:E:401:THR:HG21	1.85	0.40
1:F:200:ILE:HB	1:F:257:THR:O	2.21	0.40
1:B:314:ILE:O	1:B:314:ILE:HD12	2.21	0.40
1:C:113:ASN:HA	1:C:114:PRO:HD3	1.93	0.40
1:D:435:LEU:HD13	1:D:435:LEU:HA	1.87	0.40
1:E:408:LEU:HA	1:E:408:LEU:HD23	1.82	0.40
1:C:35:THR:C	1:C:38:PRO:HD2	2.47	0.40
1:C:286:LYS:HD3	1:D:297:HIS:NE2	2.36	0.40
1:C:297:HIS:CE1	1:D:286:LYS:CD	3.03	0.40
1:E:50:THR:HG21	1:E:86:THR:O	2.21	0.40
1:E:146:THR:C	1:E:147:ILE:HG13	2.45	0.40
1:E:214:THR:O	1:E:217:ILE:CG1	2.69	0.40
1:F:159:LEU:HD23	1:F:159:LEU:HA	1.98	0.40
1:B:155:SER:HA	1:B:364:ASN:ND2	2.37	0.40
1:C:258:VAL:HG22	1:C:259:PRO:HD3	2.03	0.40
1:E:19:ARG:O	1:E:88:ASP:HB2	2.22	0.40
1:E:258:VAL:HA	1:E:259:PRO:HD3	1.89	0.40
1:A:297:HIS:CE1	1:B:286:LYS:CD	3.04	0.40
1:B:264:PHE:CG	1:B:265:GLN:N	2.90	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	386/438 (88%)	356 (92%)	24 (6%)	6 (2%)	7	17
1	B	383/438 (87%)	353 (92%)	26 (7%)	4 (1%)	12	25
1	C	382/438 (87%)	350 (92%)	25 (6%)	7 (2%)	6	15
1	D	386/438 (88%)	352 (91%)	27 (7%)	7 (2%)	6	15
1	E	381/438 (87%)	304 (80%)	65 (17%)	12 (3%)	3	7
1	F	381/438 (87%)	298 (78%)	67 (18%)	16 (4%)	2	3
All	All	2299/2628 (88%)	2013 (88%)	234 (10%)	52 (2%)	5	11

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	433	TYR
1	C	349	ILE
1	C	378	ASN
1	C	433	TYR
1	D	124	ALA
1	E	378	ASN
1	F	378	ASN
1	D	324	THR
1	E	66	ARG
1	E	76	PRO
1	E	183	GLY
1	E	310	GLY
1	F	66	ARG
1	F	76	PRO
1	F	321	TYR
1	F	324	THR
1	A	388	GLN
1	C	388	GLN
1	E	28	ALA
1	E	309	ALA

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Mol	Chain	Res	Type
1	F	28	ALA
1	F	302	ASP
1	A	28	ALA
1	B	52	LEU
1	B	76	PRO
1	C	28	ALA
1	D	28	ALA
1	D	388	GLN
1	E	265	GLN
1	E	321	TYR
1	F	265	GLN
1	F	303	LEU
1	F	309	ALA
1	A	76	PRO
1	B	28	ALA
1	C	52	LEU
1	C	76	PRO
1	D	52	LEU
1	D	76	PRO
1	D	433	TYR
1	E	149	SER
1	E	415	VAL
1	F	149	SER
1	A	434	SER
1	F	296	ILE
1	E	296	ILE
1	F	17	PRO
1	A	430	ILE
1	F	352	VAL
1	B	430	ILE
1	F	314	ILE
1	F	55	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	338/375 (90%)	305 (90%)	33 (10%)	7	16
1	B	335/375 (89%)	302 (90%)	33 (10%)	7	16
1	C	335/375 (89%)	305 (91%)	30 (9%)	9	19
1	D	338/375 (90%)	306 (90%)	32 (10%)	8	17
1	E	333/375 (89%)	300 (90%)	33 (10%)	7	16
1	F	333/375 (89%)	307 (92%)	26 (8%)	11	25
All	All	2012/2250 (89%)	1825 (91%)	187 (9%)	8	18

All (187) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	PHE
1	A	41	LEU
1	A	58	GLU
1	A	65	GLN
1	A	67	LEU
1	A	83	SER
1	A	107	LEU
1	A	129	LEU
1	A	151	GLN
1	A	191	VAL
1	A	193	SER
1	A	197	ILE
1	A	204	VAL
1	A	217	ILE
1	A	229	ILE
1	A	243	ILE
1	A	250	LEU
1	A	252	GLN
1	A	256	LYS
1	A	258	VAL
1	A	263	LEU
1	A	347	LYS
1	A	349	ILE
1	A	367	ARG
1	A	379	THR
1	A	390	VAL
1	A	397	GLU
1	A	408	LEU
1	A	417	LYS
1	A	427	VAL

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Mol	Chain	Res	Type
1	A	428	SER
1	A	430	ILE
1	A	435	LEU
1	B	22	PHE
1	B	41	LEU
1	B	58	GLU
1	B	65	GLN
1	B	67	LEU
1	B	83	SER
1	B	107	LEU
1	B	129	LEU
1	B	151	GLN
1	B	191	VAL
1	B	193	SER
1	B	197	ILE
1	B	204	VAL
1	B	217	ILE
1	B	229	ILE
1	B	243	ILE
1	B	250	LEU
1	B	252	GLN
1	B	256	LYS
1	B	258	VAL
1	B	263	LEU
1	B	347	LYS
1	B	348	GLU
1	B	349	ILE
1	B	367	ARG
1	B	387	SER
1	B	390	VAL
1	B	397	GLU
1	B	408	LEU
1	B	417	LYS
1	B	427	VAL
1	B	428	SER
1	B	430	ILE
1	C	22	PHE
1	C	41	LEU
1	C	58	GLU
1	C	65	GLN
1	C	67	LEU
1	C	83	SER

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Mol	Chain	Res	Type
1	C	107	LEU
1	C	129	LEU
1	C	151	GLN
1	C	191	VAL
1	C	193	SER
1	C	197	ILE
1	C	204	VAL
1	C	217	ILE
1	C	229	ILE
1	C	243	ILE
1	C	250	LEU
1	C	252	GLN
1	C	258	VAL
1	C	263	LEU
1	C	347	LYS
1	C	349	ILE
1	C	367	ARG
1	C	390	VAL
1	C	397	GLU
1	C	408	LEU
1	C	417	LYS
1	C	427	VAL
1	C	428	SER
1	C	430	ILE
1	D	22	PHE
1	D	41	LEU
1	D	58	GLU
1	D	65	GLN
1	D	67	LEU
1	D	83	SER
1	D	107	LEU
1	D	129	LEU
1	D	151	GLN
1	D	191	VAL
1	D	193	SER
1	D	197	ILE
1	D	204	VAL
1	D	217	ILE
1	D	229	ILE
1	D	243	ILE
1	D	250	LEU
1	D	252	GLN

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Mol	Chain	Res	Type
1	D	256	LYS
1	D	258	VAL
1	D	263	LEU
1	D	324	THR
1	D	347	LYS
1	D	367	ARG
1	D	390	VAL
1	D	397	GLU
1	D	408	LEU
1	D	417	LYS
1	D	427	VAL
1	D	428	SER
1	D	430	ILE
1	D	435	LEU
1	E	58	GLU
1	E	67	LEU
1	E	70	SER
1	E	94	ILE
1	E	107	LEU
1	E	112	ASN
1	E	115	ASN
1	E	129	LEU
1	E	144	VAL
1	E	151	GLN
1	E	197	ILE
1	E	202	ASN
1	E	204	VAL
1	E	217	ILE
1	E	254	VAL
1	E	256	LYS
1	E	258	VAL
1	E	262	LEU
1	E	285	THR
1	E	322	SER
1	E	325	ARG
1	E	348	GLU
1	E	355	LEU
1	E	379	THR
1	E	397	GLU
1	E	401	THR
1	E	408	LEU
1	E	414	SER

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Mol	Chain	Res	Type
1	E	417	LYS
1	E	420	MET
1	E	421	MET
1	E	427	VAL
1	E	431	SER
1	F	58	GLU
1	F	67	LEU
1	F	70	SER
1	F	94	ILE
1	F	107	LEU
1	F	112	ASN
1	F	115	ASN
1	F	129	LEU
1	F	144	VAL
1	F	157	TYR
1	F	184	TRP
1	F	193	SER
1	F	204	VAL
1	F	217	ILE
1	F	254	VAL
1	F	256	LYS
1	F	258	VAL
1	F	262	LEU
1	F	285	THR
1	F	314	ILE
1	F	348	GLU
1	F	388	GLN
1	F	397	GLU
1	F	401	THR
1	F	408	LEU
1	F	421	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (111) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	46	GLN
1	A	65	GLN
1	A	112	ASN
1	A	115	ASN
1	A	131	GLN
1	A	145	GLN

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Mol	Chain	Res	Type
1	A	151	GLN
1	A	174	ASN
1	A	202	ASN
1	A	236	ASN
1	A	252	GLN
1	A	265	GLN
1	A	272	ASN
1	A	354	HIS
1	A	357	ASN
1	A	359	ASN
1	A	364	ASN
1	B	46	GLN
1	B	65	GLN
1	B	112	ASN
1	B	115	ASN
1	B	145	GLN
1	B	151	GLN
1	B	174	ASN
1	B	202	ASN
1	B	219	GLN
1	B	230	ASN
1	B	236	ASN
1	B	252	GLN
1	B	265	GLN
1	B	272	ASN
1	B	354	HIS
1	B	357	ASN
1	B	359	ASN
1	B	364	ASN
1	C	42	GLN
1	C	46	GLN
1	C	65	GLN
1	C	112	ASN
1	C	115	ASN
1	C	131	GLN
1	C	145	GLN
1	C	174	ASN
1	C	202	ASN
1	C	219	GLN
1	C	236	ASN
1	C	252	GLN
1	C	265	GLN

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Mol	Chain	Res	Type
1	C	272	ASN
1	C	354	HIS
1	C	357	ASN
1	C	359	ASN
1	C	364	ASN
1	D	42	GLN
1	D	46	GLN
1	D	65	GLN
1	D	112	ASN
1	D	115	ASN
1	D	131	GLN
1	D	145	GLN
1	D	151	GLN
1	D	174	ASN
1	D	202	ASN
1	D	219	GLN
1	D	230	ASN
1	D	236	ASN
1	D	252	GLN
1	D	265	GLN
1	D	272	ASN
1	D	354	HIS
1	D	357	ASN
1	D	359	ASN
1	D	364	ASN
1	E	48	GLN
1	E	65	GLN
1	E	99	HIS
1	E	112	ASN
1	E	115	ASN
1	E	131	GLN
1	E	145	GLN
1	E	151	GLN
1	E	174	ASN
1	E	202	ASN
1	E	236	ASN
1	E	252	GLN
1	E	265	GLN
1	E	272	ASN
1	E	354	HIS
1	E	357	ASN
1	E	364	ASN

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Mol	Chain	Res	Type
1	E	376	HIS
1	E	429	ASN
1	F	36	HIS
1	F	46	GLN
1	F	48	GLN
1	F	65	GLN
1	F	99	HIS
1	F	115	ASN
1	F	131	GLN
1	F	145	GLN
1	F	151	GLN
1	F	202	ASN
1	F	213	HIS
1	F	236	ASN
1	F	252	GLN
1	F	261	HIS
1	F	272	ASN
1	F	297	HIS
1	F	357	ASN
1	F	364	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	392/438 (89%)	0.45	15 (3%)	44	35	51, 88, 138, 216	0
1	B	389/438 (88%)	0.43	11 (2%)	55	46	53, 89, 131, 169	0
1	C	388/438 (88%)	0.58	23 (5%)	28	21	54, 93, 163, 296	0
1	D	392/438 (89%)	0.43	17 (4%)	40	31	20, 86, 131, 183	0
1	E	387/438 (88%)	1.16	62 (16%)	5	4	80, 129, 203, 281	0
1	F	387/438 (88%)	1.23	60 (15%)	5	4	74, 136, 215, 350	0
All	All	2335/2628 (88%)	0.71	188 (8%)	18	13	20, 102, 181, 350	0

All (188) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	325	ARG	5.5
1	F	47	PHE	4.8
1	C	57	ILE	4.3
1	A	30	GLY	4.2
1	F	365	ILE	4.1
1	E	294	ILE	4.1
1	F	294	ILE	4.1
1	E	365	ILE	4.0
1	A	31	TRP	4.0
1	A	72	ALA	4.0
1	F	191	VAL	4.0
1	B	73	THR	3.9
1	E	352	VAL	3.9
1	F	295	ASP	3.8
1	A	252	GLN	3.8
1	F	319	LEU	3.7
1	E	309	ALA	3.7
1	E	93	ALA	3.6
1	E	73	THR	3.6

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Mol	Chain	Res	Type	RSRZ
1	E	36	HIS	3.5
1	C	277	CYS	3.5
1	F	277	CYS	3.4
1	F	257	THR	3.4
1	C	30	GLY	3.4
1	E	293	VAL	3.4
1	E	320	TYR	3.4
1	E	321	TYR	3.4
1	C	76	PRO	3.3
1	F	352	VAL	3.2
1	D	387	SER	3.2
1	E	430	ILE	3.2
1	F	74	ALA	3.1
1	C	23	VAL	3.1
1	F	250	LEU	3.1
1	A	86	THR	3.1
1	D	16	ALA	3.0
1	C	144	VAL	3.0
1	E	16	ALA	3.0
1	A	295	ASP	3.0
1	F	278	SER	3.0
1	C	49	ILE	3.0
1	D	75	PHE	3.0
1	E	302	ASP	3.0
1	B	31	TRP	3.0
1	F	305	LEU	3.0
1	D	350	MET	3.0
1	F	86	THR	3.0
1	E	319	LEU	2.9
1	C	322	SER	2.9
1	F	251	GLY	2.9
1	B	387	SER	2.9
1	E	98	SER	2.9
1	E	305	LEU	2.9
1	D	324	THR	2.8
1	F	300	LYS	2.8
1	C	72	ALA	2.8
1	E	284	PRO	2.8
1	E	264	PHE	2.8
1	C	314	ILE	2.8
1	B	169	TYR	2.8
1	C	169	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	279	PHE	2.8
1	B	68	LYS	2.7
1	E	158	ILE	2.7
1	E	372	ILE	2.7
1	F	159	LEU	2.7
1	F	292	LEU	2.7
1	D	271	GLY	2.7
1	C	252	GLN	2.7
1	E	292	LEU	2.7
1	F	283	LYS	2.6
1	F	312	ALA	2.6
1	E	369	TYR	2.6
1	F	25	LEU	2.6
1	E	312	ALA	2.6
1	F	279	PHE	2.6
1	E	358	TYR	2.6
1	E	304	LYS	2.6
1	C	63	THR	2.6
1	D	73	THR	2.6
1	E	30	GLY	2.6
1	E	183	GLY	2.6
1	F	284	PRO	2.6
1	E	277	CYS	2.6
1	B	15	ALA	2.6
1	F	119	LEU	2.5
1	E	310	GLY	2.5
1	E	278	SER	2.5
1	C	420	MET	2.5
1	E	125	LEU	2.5
1	D	27	ALA	2.5
1	F	150	LEU	2.5
1	A	301	GLY	2.5
1	F	276	SER	2.5
1	F	369	TYR	2.5
1	F	48	GLN	2.5
1	F	303	LEU	2.4
1	C	309	ALA	2.4
1	F	354	HIS	2.4
1	C	350	MET	2.4
1	E	296	ILE	2.4
1	F	57	ILE	2.4
1	F	90	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	50	THR	2.4
1	D	144	VAL	2.4
1	E	295	ASP	2.4
1	F	62	ALA	2.4
1	F	197	ILE	2.4
1	E	102	VAL	2.4
1	D	309	ALA	2.4
1	E	157	TYR	2.4
1	F	293	VAL	2.3
1	A	48	GLN	2.3
1	D	20	VAL	2.3
1	F	183	GLY	2.3
1	C	295	ASP	2.3
1	B	74	ALA	2.3
1	B	309	ALA	2.3
1	F	309	ALA	2.3
1	E	89	MET	2.3
1	D	31	TRP	2.3
1	D	84	SER	2.3
1	C	73	THR	2.3
1	E	57	ILE	2.3
1	E	349	ILE	2.3
1	E	353	TYR	2.3
1	E	379	THR	2.3
1	D	347	LYS	2.3
1	E	350	MET	2.3
1	C	321	TYR	2.3
1	F	254	VAL	2.3
1	F	288	PHE	2.3
1	F	242	LEU	2.3
1	F	61	ILE	2.3
1	F	285	THR	2.3
1	E	282	GLY	2.3
1	B	350	MET	2.2
1	D	74	ALA	2.2
1	F	34	LYS	2.2
1	F	161	ALA	2.2
1	A	417	LYS	2.2
1	E	299	THR	2.2
1	F	144	VAL	2.2
1	E	371	SER	2.2
1	F	227	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	23	VAL	2.2
1	A	387	SER	2.2
1	E	37	TYR	2.2
1	F	310	GLY	2.2
1	E	283	LYS	2.2
1	E	191	VAL	2.2
1	F	204	VAL	2.2
1	F	302	ASP	2.2
1	B	310	GLY	2.2
1	F	286	LYS	2.2
1	A	194	PRO	2.1
1	C	31	TRP	2.1
1	E	184	TRP	2.1
1	E	164	LEU	2.1
1	E	355	LEU	2.1
1	C	315	SER	2.1
1	D	70	SER	2.1
1	E	247	GLY	2.1
1	F	353	TYR	2.1
1	E	25	LEU	2.1
1	E	288	PHE	2.1
1	E	176	ILE	2.1
1	A	60	SER	2.1
1	F	350	MET	2.1
1	E	207	VAL	2.1
1	B	349	ILE	2.1
1	A	177	GLU	2.1
1	A	169	TYR	2.1
1	E	118	TYR	2.1
1	F	431	SER	2.0
1	A	71	ASN	2.0
1	F	164	LEU	2.0
1	F	211	PHE	2.0
1	F	307	GLY	2.0
1	F	398	GLY	2.0
1	C	116	LEU	2.0
1	E	218	LEU	2.0
1	E	49	ILE	2.0
1	F	170	ILE	2.0
1	E	221	MET	2.0
1	F	123	TRP	2.0
1	C	369	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	23	VAL	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 oligosaccharides 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.