



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:40 AM UTC

PDB ID : 3P16 / pdb_00003p16
Title : Crystal structure of DNA polymerase III sliding clamp
Authors : Gui, W.J.; Lin, S.Q.; Chen, Y.Y.; Zhang, X.E.; Bi, L.J.; Jiang, T.
Deposited on : 2010-09-30
Resolution : 2.89 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

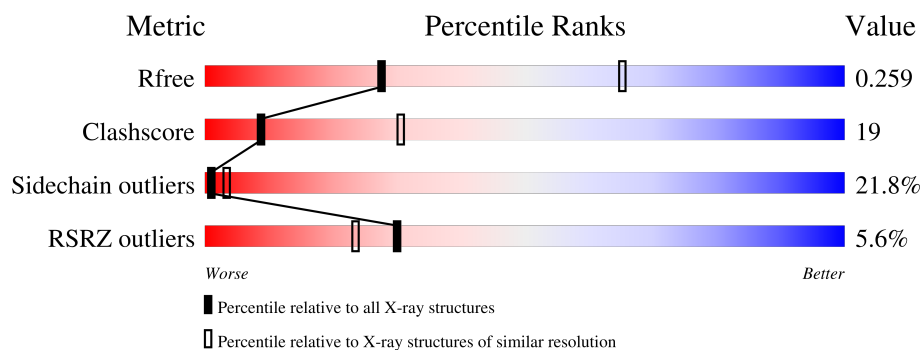
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	408	5% 54% 38% 8%
1	B	408	4% 60% 31% 6%
1	C	408	6% 55% 28% 8% 9%
1	D	408	4% 54% 31% 5% 10%
1	E	408	5% 52% 30% 9% 10%
1	F	408	7% 51% 33% 7% 9%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 16587 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 DNA polymerase III subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	375	Total	C	N	O	S	0	0	0
			2776	1755	474	541	6			
1	B	383	Total	C	N	O	S	0	0	0
			2836	1796	485	549	6			
1	C	370	Total	C	N	O	S	0	0	0
			2744	1737	469	532	6			
1	D	369	Total	C	N	O	S	0	0	0
			2738	1734	468	530	6			
1	E	369	Total	C	N	O	S	0	0	0
			2738	1734	468	530	6			
1	F	372	Total	C	N	O	S	0	0	0
			2755	1744	471	534	6			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP Q50790
A	-4	HIS	-	expression tag	UNP Q50790
A	-3	HIS	-	expression tag	UNP Q50790
A	-2	HIS	-	expression tag	UNP Q50790
A	-1	HIS	-	expression tag	UNP Q50790
A	0	HIS	-	expression tag	UNP Q50790
B	-5	HIS	-	expression tag	UNP Q50790
B	-4	HIS	-	expression tag	UNP Q50790
B	-3	HIS	-	expression tag	UNP Q50790
B	-2	HIS	-	expression tag	UNP Q50790
B	-1	HIS	-	expression tag	UNP Q50790
B	0	HIS	-	expression tag	UNP Q50790
C	-5	HIS	-	expression tag	UNP Q50790
C	-4	HIS	-	expression tag	UNP Q50790
C	-3	HIS	-	expression tag	UNP Q50790
C	-2	HIS	-	expression tag	UNP Q50790
C	-1	HIS	-	expression tag	UNP Q50790

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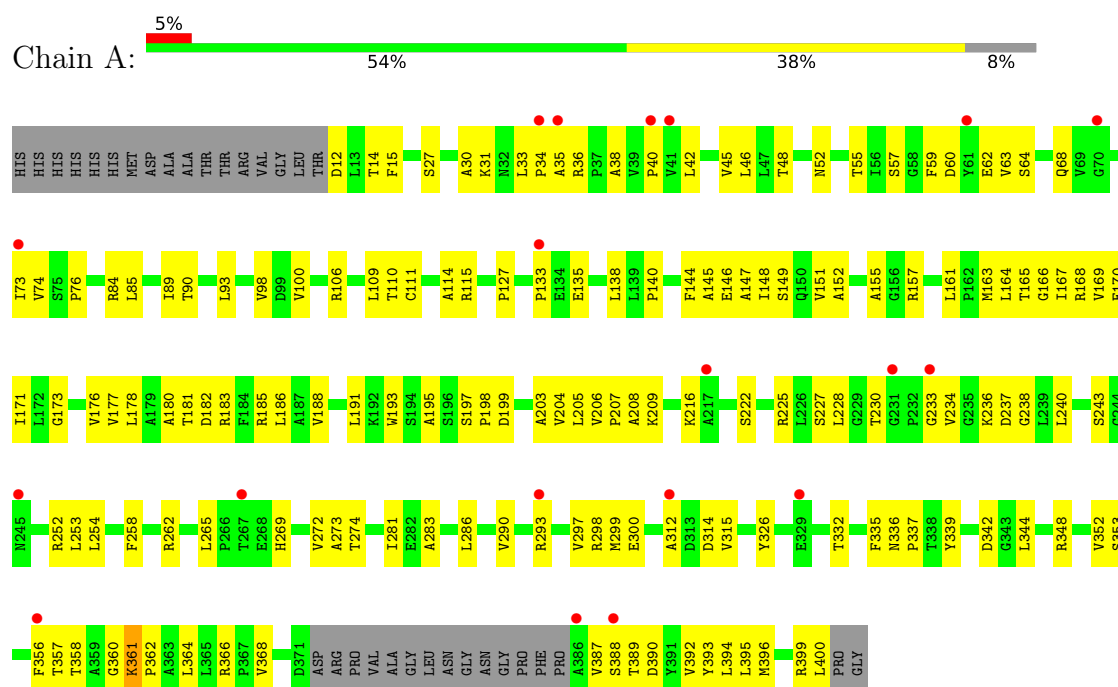
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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	HIS	-	expression tag	UNP Q50790
D	-5	HIS	-	expression tag	UNP Q50790
D	-4	HIS	-	expression tag	UNP Q50790
D	-3	HIS	-	expression tag	UNP Q50790
D	-2	HIS	-	expression tag	UNP Q50790
D	-1	HIS	-	expression tag	UNP Q50790
D	0	HIS	-	expression tag	UNP Q50790
E	-5	HIS	-	expression tag	UNP Q50790
E	-4	HIS	-	expression tag	UNP Q50790
E	-3	HIS	-	expression tag	UNP Q50790
E	-2	HIS	-	expression tag	UNP Q50790
E	-1	HIS	-	expression tag	UNP Q50790
E	0	HIS	-	expression tag	UNP Q50790
F	-5	HIS	-	expression tag	UNP Q50790
F	-4	HIS	-	expression tag	UNP Q50790
F	-3	HIS	-	expression tag	UNP Q50790
F	-2	HIS	-	expression tag	UNP Q50790
F	-1	HIS	-	expression tag	UNP Q50790
F	0	HIS	-	expression tag	UNP Q50790

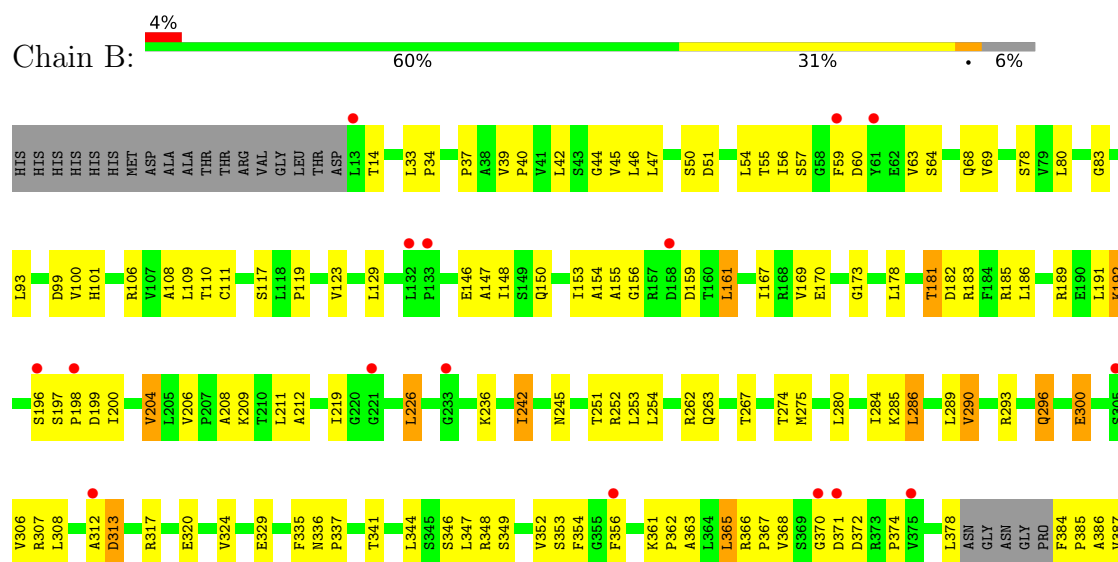
3 Residue-property plots

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: DNA polymerase III subunit beta

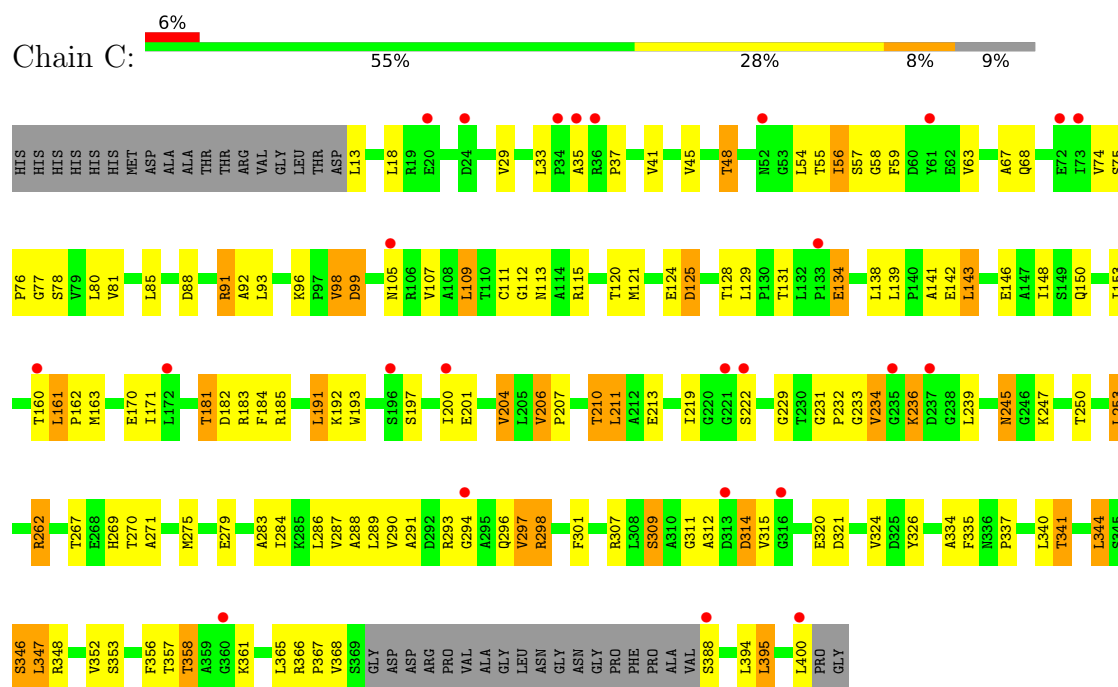


• Molecule 1: DNA polymerase III subunit beta

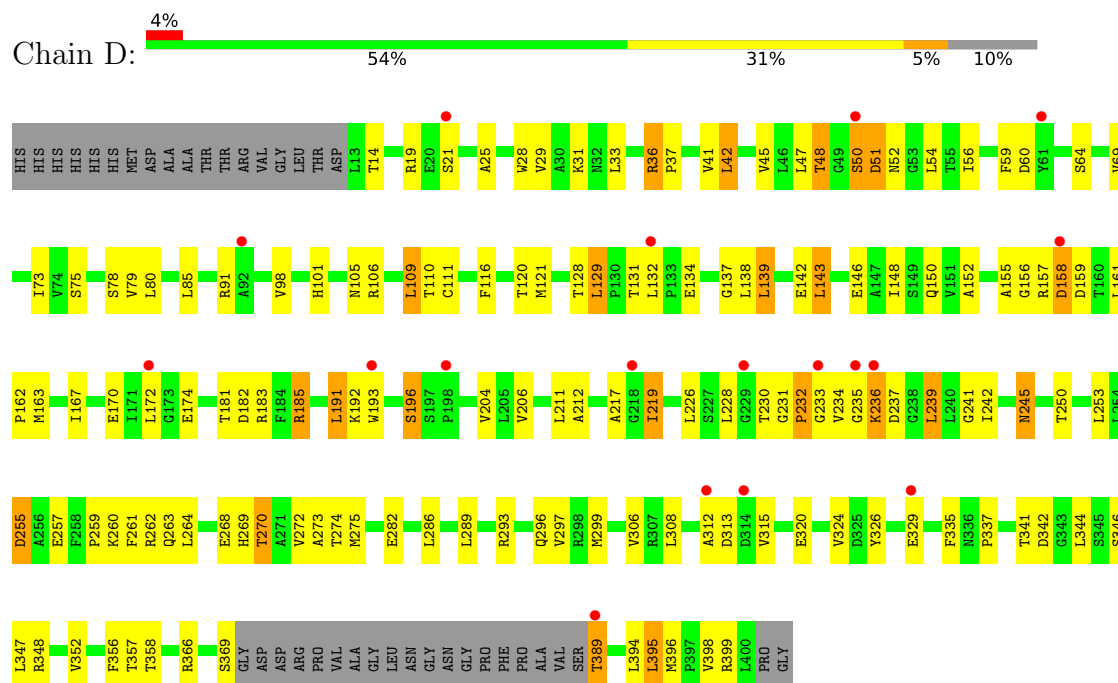




• Molecule 1: DNA polymerase III subunit beta

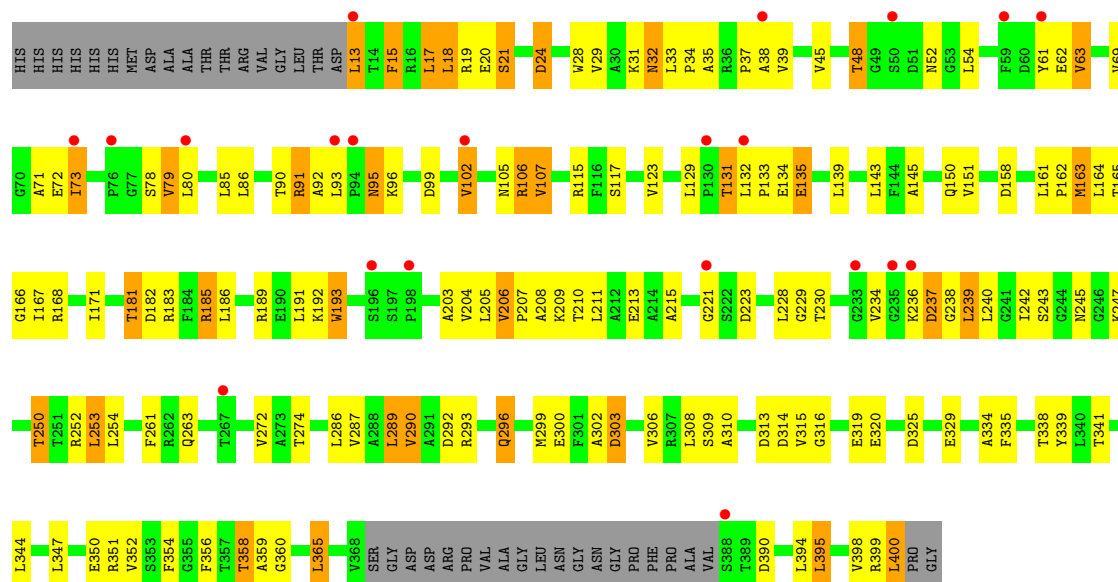


• Molecule 1: DNA polymerase III subunit beta

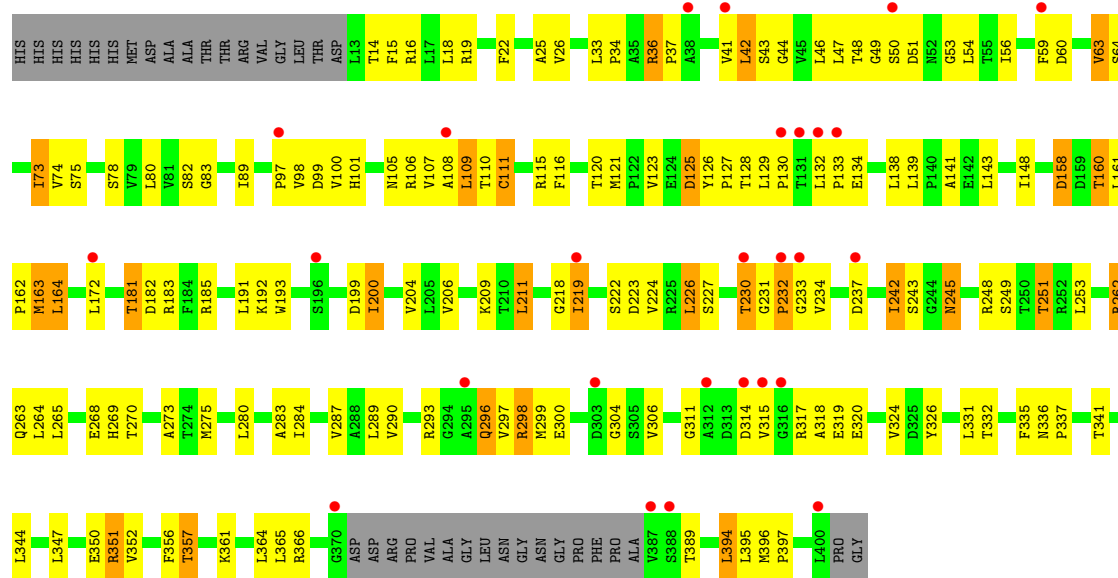


• Molecule 1: DNA polymerase III subunit beta





• Molecule 1: DNA polymerase III subunit beta



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	88.05Å 132.97Å 113.78Å 90.00° 109.05° 90.00°	Depositor
Resolution (Å)	50.00 – 2.89 50.00 – 2.89	Depositor EDS
% Data completeness (in resolution range)	97.7 (50.00-2.89) 97.7 (50.00-2.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.260 , 0.287 (Not available) , 0.259	Depositor DCC
R_{free} test set	2746 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	59.4	Xtriage
Anisotropy	0.277	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 49.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	16587	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.67	0/2821	0.96	2/3845 (0.1%)
1	B	0.61	0/2884	0.95	6/3932 (0.2%)
1	C	0.61	0/2789	0.95	3/3801 (0.1%)
1	D	0.58	0/2783	0.90	3/3793 (0.1%)
1	E	0.67	0/2783	0.96	4/3793 (0.1%)
1	F	0.63	1/2800 (0.0%)	0.95	4/3816 (0.1%)
All	All	0.63	1/16860 (0.0%)	0.94	22/22980 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	296	GLN	CA-C	5.42	1.55	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	296	GLN	N-CA-C	6.77	119.45	108.76
1	B	181	THR	N-CA-C	6.73	119.35	108.32
1	E	15	PHE	N-CA-C	6.53	118.78	108.79
1	C	181	THR	N-CA-C	6.32	119.00	108.13
1	B	161	LEU	CA-C-N	5.83	125.97	119.32
1	B	161	LEU	C-N-CA	5.83	125.97	119.32
1	F	15	PHE	N-CA-C	5.54	117.27	108.79
1	E	390	ASP	N-CA-C	-5.47	106.97	113.97
1	D	232	PRO	N-CA-C	-5.43	104.98	113.78
1	D	196	SER	N-CA-C	-5.40	106.20	112.89
1	E	181	THR	CB-CA-C	-5.33	99.82	110.42
1	D	139	LEU	N-CA-C	5.31	113.00	108.22
1	E	193	TRP	N-CA-C	5.24	117.22	108.99
1	B	336	ASN	CA-C-N	5.22	126.36	119.84
1	B	336	ASN	C-N-CA	5.22	126.36	119.84
1	F	296	GLN	N-CA-C	5.19	116.38	108.12
1	A	361	LYS	CA-C-N	5.12	125.11	119.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	361	LYS	C-N-CA	5.12	125.11	119.89
1	F	232	PRO	N-CA-C	-5.11	106.13	113.75
1	F	181	THR	CB-CA-C	-5.05	100.36	110.42
1	C	181	THR	CB-CA-C	-5.05	102.87	110.24
1	C	312	ALA	N-CA-C	5.02	115.16	108.23

There are no chirality outliers.

There are no planarity outliers.

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	2776	0	2826	165	0
1	B	2836	0	2890	92	0
1	C	2744	0	2801	79	0
1	D	2738	0	2796	93	0
1	E	2738	0	2796	121	0
1	F	2755	0	2813	105	0
All	All	16587	0	16922	626	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 19.

All (626) 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:E:234:VAL:HG11	1:E:236:LYS:NZ	1.48	1.28
1:A:30:ALA:HA	1:A:34:PRO:HG2	1.24	1.16
1:A:161:LEU:HD12	1:A:161:LEU:H	1.01	1.15
1:E:234:VAL:HG22	1:E:236:LYS:HG3	1.23	1.11
1:E:134:GLU:OE1	1:E:230:THR:HG22	1.49	1.08
1:E:234:VAL:HG11	1:E:236:LYS:CE	1.84	1.07
1:F:36:ARG:HD2	1:F:36:ARG:N	1.67	1.04
1:F:296:GLN:HB3	1:F:337:PRO:HD3	1.38	1.04
1:A:185:ARG:HD3	1:A:339:TYR:HB3	1.37	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:LEU:HD21	1:B:60:ASP:HA	1.41	1.02
1:E:234:VAL:HG21	1:E:236:LYS:HE3	1.37	1.01
1:E:234:VAL:CG2	1:E:236:LYS:HG3	1.91	1.00
1:E:206:VAL:HG23	1:E:207:PRO:HD2	1.44	1.00
1:B:280:LEU:O	1:B:284:ILE:HG12	1.61	0.99
1:C:298:ARG:HG2	1:C:298:ARG:HH11	1.27	0.97
1:D:59:PHE:CD1	1:D:64:SER:HB3	2.00	0.96
1:A:35:ALA:HA	1:A:84:ARG:HE	1.34	0.93
1:F:36:ARG:HD2	1:F:36:ARG:H	1.26	0.93
1:D:59:PHE:HD1	1:D:64:SER:HB3	1.28	0.92
1:E:145:ALA:HA	1:E:215:ALA:HB1	1.52	0.92
1:E:234:VAL:HG11	1:E:236:LYS:HZ2	1.35	0.91
1:A:387:VAL:HG22	1:A:388:SER:H	1.37	0.89
1:A:161:LEU:HD11	1:C:183:ARG:C	1.99	0.88
1:F:37:PRO:HG2	1:F:43:SER:HB3	1.55	0.88
1:B:349:SER:HB2	1:B:367:PRO:HB3	1.56	0.88
1:A:161:LEU:HD12	1:A:161:LEU:N	1.85	0.87
1:A:73:ILE:HD13	1:A:73:ILE:H	1.38	0.86
1:A:161:LEU:H	1:A:161:LEU:CD1	1.87	0.86
1:D:59:PHE:HD1	1:D:64:SER:CB	1.88	0.86
1:A:204:VAL:HG22	1:A:253:LEU:HD13	1.59	0.85
1:E:20:GLU:H	1:E:20:GLU:CD	1.84	0.85
1:F:80:LEU:HD23	1:F:121:MET:HB2	1.58	0.85
1:A:155:ALA:O	1:A:157:ARG:HG3	1.76	0.84
1:E:48:THR:HG23	1:E:78:SER:HB3	1.58	0.84
1:E:354:PHE:HB3	1:E:356:PHE:CE2	2.13	0.84
1:A:59:PHE:HB3	1:A:64:SER:HA	1.59	0.83
1:A:100:VAL:HG22	1:A:109:LEU:HD13	1.59	0.82
1:B:354:PHE:HB3	1:B:356:PHE:CE2	2.14	0.82
1:A:27:SER:O	1:A:31:LYS:HG2	1.80	0.81
1:F:337:PRO:O	1:F:341:THR:HG22	1.80	0.81
1:B:335:PHE:HZ	1:B:356:PHE:HE1	1.27	0.81
1:A:161:LEU:CD1	1:C:183:ARG:O	2.29	0.80
1:F:164:LEU:HG	1:F:181:THR:O	1.81	0.80
1:B:199:ASP:C	1:B:200:ILE:HG22	2.05	0.80
1:D:366:ARG:HD2	1:D:389:THR:HG21	1.64	0.80
1:A:157:ARG:HD2	1:A:157:ARG:O	1.81	0.79
1:E:234:VAL:HG13	1:E:236:LYS:HD2	1.63	0.78
1:E:61:TYR:HD1	1:E:62:GLU:HG2	1.48	0.78
1:E:132:LEU:N	1:E:133:PRO:HD3	1.99	0.77
1:D:19:ARG:HH21	1:D:91:ARG:HA	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:234:VAL:CG1	1:E:236:LYS:NZ	2.41	0.77
1:A:185:ARG:HD2	1:A:393:TYR:OH	1.83	0.77
1:D:366:ARG:CD	1:D:389:THR:HG21	2.15	0.76
1:E:234:VAL:CG1	1:E:236:LYS:HD2	2.16	0.76
1:E:234:VAL:HG11	1:E:236:LYS:HZ1	1.49	0.76
1:E:335:PHE:CD1	1:E:395:LEU:HD13	2.21	0.75
1:A:133:PRO:O	1:A:227:SER:HB3	1.86	0.75
1:E:204:VAL:CG2	1:E:253:LEU:HG	2.17	0.75
1:B:399:ARG:HG3	1:B:400:LEU:HG	1.68	0.75
1:F:181:THR:O	1:F:181:THR:HG23	1.86	0.74
1:F:218:GLY:HA2	1:F:245:ASN:HD21	1.51	0.74
1:D:234:VAL:O	1:D:236:LYS:N	2.21	0.74
1:A:161:LEU:CD1	1:C:183:ARG:C	2.60	0.74
1:A:161:LEU:HD12	1:C:183:ARG:O	1.87	0.73
1:A:300:GLU:HG3	1:A:332:THR:OG1	1.87	0.73
1:A:297:VAL:HG23	1:A:337:PRO:HG3	1.70	0.73
1:A:315:VAL:HA	1:B:119:PRO:HG2	1.70	0.73
1:D:268:GLU:HG3	1:D:269:HIS:H	1.54	0.73
1:D:270:THR:HB	1:D:357:THR:HA	1.68	0.73
1:F:109:LEU:HB3	1:F:116:PHE:HB2	1.71	0.72
1:F:218:GLY:CA	1:F:245:ASN:HD21	2.02	0.72
1:E:181:THR:OG1	1:E:182:ASP:O	2.07	0.72
1:B:40:PRO:HG3	1:D:36:ARG:HH11	1.53	0.72
1:A:144:PHE:O	1:A:148:ILE:HG13	1.89	0.72
1:E:73:ILE:O	1:E:73:ILE:HG13	1.89	0.72
1:C:233:GLY:O	1:C:236:LYS:HB2	1.90	0.72
1:B:354:PHE:HB3	1:B:356:PHE:HE2	1.53	0.72
1:D:260:LYS:HD3	1:D:263:GLN:HE22	1.55	0.72
1:E:234:VAL:CG2	1:E:236:LYS:CG	2.68	0.71
1:A:273:ALA:HB2	1:A:326:TYR:HD1	1.54	0.71
1:C:170:GLU:OE1	1:C:262:ARG:NH2	2.23	0.71
1:A:185:ARG:HD3	1:A:339:TYR:CB	2.15	0.71
1:B:198:PRO:O	1:B:200:ILE:HG22	1.91	0.70
1:E:134:GLU:HB3	1:E:229:GLY:HA2	1.72	0.70
1:A:389:THR:CG2	1:A:390:ASP:H	2.04	0.70
1:A:59:PHE:CZ	1:A:127:PRO:HB2	2.27	0.70
1:B:199:ASP:O	1:B:200:ILE:CG2	2.40	0.70
1:A:364:LEU:HD11	1:A:392:VAL:CG2	2.21	0.70
1:A:387:VAL:HG22	1:A:388:SER:N	2.07	0.70
1:A:387:VAL:CG2	1:A:388:SER:H	2.05	0.70
1:D:268:GLU:HG3	1:D:269:HIS:N	2.07	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:VAL:HG23	1:A:167:ILE:HD13	1.73	0.69
1:A:181:THR:HB	1:A:186:LEU:HA	1.74	0.69
1:A:238:GLY:O	1:A:252:ARG:HA	1.92	0.69
1:F:25:ALA:HB1	1:F:56:ILE:HD12	1.73	0.69
1:A:55:THR:HG22	1:A:68:GLN:HB2	1.73	0.69
1:E:234:VAL:HG22	1:E:236:LYS:CG	2.13	0.69
1:A:15:PHE:HB3	1:A:73:ILE:HG22	1.75	0.68
1:A:389:THR:HG22	1:A:390:ASP:H	1.58	0.68
1:B:37:PRO:HB3	1:C:314:ASP:HB2	1.76	0.68
1:E:234:VAL:CG1	1:E:236:LYS:CE	2.67	0.68
1:D:59:PHE:CD1	1:D:64:SER:CB	2.69	0.68
1:A:36:ARG:HH12	1:A:38:ALA:CB	2.07	0.68
1:B:199:ASP:C	1:B:200:ILE:CG2	2.66	0.68
1:A:140:PRO:HA	1:A:222:SER:HA	1.75	0.67
1:B:293:ARG:CG	1:B:293:ARG:O	2.43	0.67
1:D:25:ALA:HB1	1:D:56:ILE:HD13	1.77	0.67
1:E:234:VAL:CG2	1:E:236:LYS:HE3	2.21	0.67
1:B:150:GLN:OE1	1:B:189:ARG:HD3	1.95	0.66
1:A:147:ALA:HB1	1:A:178:LEU:HD12	1.78	0.66
1:C:57:SER:HB3	1:C:129:LEU:HD11	1.77	0.66
1:D:274:THR:O	1:D:324:VAL:HG23	1.95	0.66
1:E:238:GLY:O	1:E:252:ARG:HA	1.95	0.66
1:F:46:LEU:HD11	1:F:123:VAL:HG13	1.76	0.66
1:E:61:TYR:CD1	1:E:62:GLU:HG2	2.31	0.65
1:A:206:VAL:HG21	1:A:240:LEU:HD12	1.79	0.65
1:C:197:SER:O	1:C:200:ILE:HG12	1.97	0.65
1:C:29:VAL:HG21	1:C:56:ILE:O	1.96	0.65
1:A:35:ALA:HA	1:A:84:ARG:NE	2.10	0.65
1:D:183:ARG:HB3	1:F:160:THR:HG23	1.78	0.65
1:F:364:LEU:HD21	1:F:366:ARG:HH21	1.60	0.65
1:B:54:LEU:C	1:B:54:LEU:HD13	2.21	0.64
1:B:54:LEU:HD12	1:B:69:VAL:HG12	1.79	0.64
1:E:234:VAL:HG21	1:E:236:LYS:CE	2.20	0.64
1:A:389:THR:HG22	1:A:390:ASP:N	2.12	0.64
1:A:36:ARG:NH1	1:A:38:ALA:HB3	2.12	0.64
1:D:293:ARG:HH22	1:F:293:ARG:NH1	1.96	0.64
1:F:49:GLY:O	1:F:73:ILE:HD13	1.98	0.64
1:F:51:ASP:C	1:F:53:GLY:H	2.06	0.64
1:B:54:LEU:HD11	1:B:56:ILE:HD11	1.80	0.63
1:E:86:LEU:O	1:E:90:THR:HG23	1.97	0.63
1:B:366:ARG:CZ	1:B:387:VAL:HG21	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:HIS:CD2	1:A:272:VAL:CG1	2.82	0.63
1:B:148:ILE:HG21	1:B:212:ALA:HA	1.80	0.62
1:F:141:ALA:HB1	1:F:219:ILE:O	1.99	0.62
1:E:354:PHE:CB	1:E:356:PHE:CE2	2.82	0.62
1:A:114:ALA:HB2	1:B:320:GLU:HG2	1.81	0.62
1:B:386:ALA:O	1:B:387:VAL:HG13	1.99	0.62
1:E:234:VAL:CG1	1:E:236:LYS:CD	2.77	0.62
1:F:231:GLY:O	1:F:234:VAL:HG13	1.98	0.62
1:A:164:LEU:HD23	1:A:164:LEU:H	1.65	0.62
1:D:129:LEU:HD22	1:D:129:LEU:H	1.65	0.62
1:F:16:ARG:HD2	1:F:97:PRO:HB2	1.81	0.62
1:D:36:ARG:N	1:D:37:PRO:HD2	2.15	0.62
1:A:135:GLU:OE1	1:A:225:ARG:HD3	2.00	0.61
1:B:14:THR:HG23	1:B:101:HIS:HB3	1.83	0.61
1:B:356:PHE:CE1	1:B:363:ALA:CB	2.83	0.61
1:E:20:GLU:OE2	1:E:95:ASN:HB3	2.01	0.61
1:C:298:ARG:HH11	1:C:298:ARG:CG	2.08	0.61
1:B:173:GLY:HA2	1:B:200:ILE:HG23	1.81	0.61
1:D:146:GLU:O	1:D:150:GLN:HG3	2.00	0.61
1:E:31:LYS:HD2	1:E:213:GLU:HG3	1.82	0.61
1:C:207:PRO:HB2	1:C:210:THR:HG23	1.83	0.61
1:A:205:LEU:O	1:A:253:LEU:HB2	2.01	0.60
1:E:204:VAL:HG22	1:E:253:LEU:HG	1.82	0.60
1:A:389:THR:CG2	1:A:390:ASP:N	2.65	0.60
1:B:293:ARG:O	1:B:293:ARG:HG3	2.01	0.60
1:D:312:ALA:HB3	1:D:315:VAL:HB	1.83	0.60
1:E:134:GLU:CD	1:E:230:THR:H	2.09	0.60
1:B:199:ASP:O	1:B:200:ILE:HG22	2.00	0.60
1:B:156:GLY:HA2	1:B:182:ASP:HB3	1.83	0.59
1:B:353:SER:HB3	1:B:366:ARG:HG3	1.82	0.59
1:D:293:ARG:HH22	1:F:293:ARG:HH11	1.49	0.59
1:A:12:ASP:O	1:A:76:PRO:O	2.20	0.59
1:F:41:VAL:HG13	1:F:126:TYR:HD1	1.67	0.59
1:B:55:THR:HG23	1:B:68:GLN:HG2	1.84	0.59
1:E:13:LEU:O	1:E:102:VAL:HG13	2.02	0.59
1:F:226:LEU:HD12	1:F:242:ILE:HG22	1.83	0.59
1:F:269:HIS:HB3	1:F:356:PHE:O	2.03	0.59
1:A:42:LEU:HD21	1:A:60:ASP:HA	1.84	0.59
1:E:234:VAL:CG1	1:E:236:LYS:HZ2	2.08	0.59
1:A:36:ARG:HH12	1:A:38:ALA:HB3	1.65	0.59
1:C:298:ARG:HG2	1:C:298:ARG:NH1	2.06	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:354:PHE:CD1	1:B:356:PHE:CZ	2.91	0.58
1:E:33:LEU:N	1:E:34:PRO:HD3	2.18	0.58
1:A:106:ARG:CG	1:A:106:ARG:HH11	2.15	0.58
1:D:132:LEU:HD13	1:D:241:GLY:HA3	1.84	0.58
1:E:234:VAL:HG11	1:E:236:LYS:CD	2.32	0.58
1:B:356:PHE:CE1	1:B:363:ALA:HB2	2.38	0.58
1:C:80:LEU:HD23	1:C:121:MET:HB2	1.85	0.58
1:A:33:LEU:HD23	1:A:63:VAL:HG13	1.86	0.58
1:C:181:THR:O	1:C:181:THR:HG23	2.03	0.58
1:A:163:MET:O	1:A:164:LEU:C	2.45	0.58
1:A:144:PHE:O	1:A:148:ILE:CG1	2.52	0.58
1:D:157:ARG:O	1:D:158:ASP:C	2.47	0.58
1:E:315:VAL:HG13	1:F:106:ARG:HH12	1.68	0.58
1:A:40:PRO:C	1:A:42:LEU:H	2.12	0.57
1:C:201:GLU:O	1:C:234:VAL:HG13	2.04	0.57
1:A:73:ILE:HD13	1:A:73:ILE:N	2.15	0.57
1:A:181:THR:HG22	1:A:258:PHE:CZ	2.39	0.57
1:E:228:LEU:O	1:E:234:VAL:O	2.21	0.57
1:F:48:THR:HG22	1:F:50:SER:H	1.69	0.57
1:C:109:LEU:HD12	1:C:109:LEU:C	2.29	0.57
1:E:296:GLN:HE21	1:E:400:LEU:HD22	1.69	0.57
1:B:59:PHE:CD2	1:B:64:SER:HB3	2.40	0.57
1:C:269:HIS:HB3	1:C:356:PHE:O	2.05	0.57
1:C:141:ALA:H	1:C:222:SER:HA	1.69	0.56
1:A:62:GLU:HA	1:A:252:ARG:HG3	1.88	0.56
1:A:110:THR:HG22	1:A:115:ARG:HG3	1.87	0.56
1:A:46:LEU:HB3	1:A:57:SER:HB2	1.87	0.56
1:D:268:GLU:CG	1:D:269:HIS:H	2.17	0.56
1:D:219:ILE:HG12	1:D:219:ILE:O	2.04	0.56
1:C:81:VAL:HG11	1:C:107:VAL:HG11	1.87	0.56
1:B:59:PHE:HB2	1:B:129:LEU:HD22	1.87	0.56
1:A:170:GLU:HG3	1:A:177:VAL:HB	1.87	0.56
1:E:131:THR:C	1:E:133:PRO:HD3	2.31	0.56
1:F:283:ALA:O	1:F:287:VAL:HG22	2.06	0.55
1:B:374:PRO:HD2	1:B:388:SER:HB3	1.88	0.55
1:C:207:PRO:HB2	1:C:210:THR:CG2	2.37	0.55
1:A:269:HIS:HD2	1:A:272:VAL:CG1	2.19	0.55
1:A:145:ALA:O	1:A:149:SER:HB2	2.07	0.55
1:C:48:THR:HG23	1:C:78:SER:HB3	1.88	0.55
1:A:197:SER:HB2	1:A:230:THR:HG22	1.88	0.55
1:D:159:ASP:C	1:D:161:LEU:H	2.13	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:LEU:HD11	1:A:392:VAL:HG22	1.87	0.55
1:C:161:LEU:HD23	1:C:162:PRO:HD2	1.88	0.55
1:F:49:GLY:O	1:F:73:ILE:CD1	2.55	0.55
1:B:335:PHE:CZ	1:B:356:PHE:HE1	2.16	0.54
1:B:398:VAL:HG12	1:B:399:ARG:N	2.22	0.54
1:C:337:PRO:O	1:C:341:THR:HB	2.07	0.54
1:D:185:ARG:HA	1:D:394:LEU:O	2.07	0.54
1:F:219:ILE:HD13	1:F:219:ILE:C	2.31	0.54
1:D:335:PHE:CD1	1:D:395:LEU:HD13	2.42	0.54
1:A:168:ARG:HH12	1:A:203:ALA:HB1	1.72	0.54
1:A:59:PHE:HB3	1:A:64:SER:CA	2.35	0.54
1:A:225:ARG:HB3	1:A:243:SER:HB2	1.90	0.54
1:B:192:LYS:H	1:B:192:LYS:HD3	1.73	0.54
1:C:35:ALA:O	1:C:37:PRO:HD3	2.07	0.54
1:C:335:PHE:CD1	1:C:395:LEU:HD13	2.42	0.54
1:B:361:LYS:HB3	1:B:362:PRO:HD2	1.88	0.54
1:B:199:ASP:O	1:B:200:ILE:HG23	2.07	0.54
1:A:161:LEU:HD11	1:C:184:PHE:N	2.23	0.54
1:A:314:ASP:OD2	1:A:315:VAL:N	2.40	0.54
1:A:335:PHE:CD1	1:A:395:LEU:HD13	2.42	0.54
1:F:181:THR:O	1:F:181:THR:CG2	2.56	0.54
1:A:399:ARG:H	1:A:399:ARG:HE	1.55	0.53
1:A:399:ARG:H	1:A:399:ARG:NE	2.06	0.53
1:B:39:VAL:HG23	1:B:42:LEU:HB2	1.89	0.53
1:A:168:ARG:HA	1:A:205:LEU:HD12	1.89	0.53
1:B:356:PHE:CE1	1:B:363:ALA:HB1	2.43	0.53
1:E:300:GLU:O	1:E:306:VAL:HA	2.09	0.53
1:D:36:ARG:HG3	1:D:37:PRO:HD3	1.90	0.53
1:E:132:LEU:N	1:E:133:PRO:CD	2.70	0.53
1:A:33:LEU:HD11	1:A:60:ASP:HB3	1.89	0.53
1:A:233:GLY:C	1:A:234:VAL:HG13	2.33	0.53
1:A:33:LEU:HG	1:A:63:VAL:O	2.08	0.53
1:C:143:LEU:HD13	1:C:191:LEU:CD2	2.39	0.53
1:D:50:SER:O	1:D:51:ASP:C	2.52	0.53
1:E:21:SER:OG	1:E:69:VAL:HG21	2.09	0.53
1:A:42:LEU:HD23	1:A:42:LEU:O	2.09	0.53
1:A:85:LEU:O	1:A:89:ILE:HG13	2.09	0.53
1:A:170:GLU:CG	1:A:177:VAL:HB	2.39	0.53
1:B:169:VAL:HB	1:B:204:VAL:HG12	1.91	0.53
1:B:267:THR:O	1:B:386:ALA:HB2	2.09	0.53
1:C:231:GLY:O	1:C:234:VAL:HG12	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:139:LEU:HD22	1:D:193:TRP:HE1	1.74	0.52
1:F:98:VAL:HG12	1:F:111:CYS:SG	2.49	0.52
1:C:88:ASP:HB3	1:D:289:LEU:HD22	1.91	0.52
1:E:338:THR:O	1:E:341:THR:HG22	2.09	0.52
1:C:245:ASN:ND2	1:C:245:ASN:H	2.06	0.52
1:F:44:GLY:HA2	1:F:83:GLY:H	1.74	0.52
1:F:231:GLY:H	1:F:234:VAL:HG12	1.75	0.52
1:B:93:LEU:HD22	1:B:111:CYS:HB3	1.92	0.52
1:B:99:ASP:O	1:B:109:LEU:HA	2.10	0.52
1:D:181:THR:OG1	1:D:182:ASP:O	2.17	0.52
1:D:245:ASN:O	1:D:245:ASN:ND2	2.40	0.52
1:E:106:ARG:HD3	1:E:117:SER:OG	2.10	0.52
1:A:353:SER:HB2	1:A:368:VAL:CG2	2.40	0.52
1:E:17:LEU:C	1:E:18:LEU:HD13	2.35	0.52
1:F:243:SER:CB	1:F:248:ARG:HB3	2.39	0.52
1:A:33:LEU:HD21	1:A:60:ASP:CG	2.36	0.51
1:C:55:THR:HG22	1:C:68:GLN:HG2	1.92	0.51
1:B:159:ASP:C	1:B:161:LEU:H	2.17	0.51
1:D:98:VAL:HG12	1:D:111:CYS:HB2	1.91	0.51
1:E:106:ARG:HH11	1:E:106:ARG:CG	2.23	0.51
1:E:19:ARG:HD3	1:E:19:ARG:C	2.35	0.51
1:A:146:GLU:HG3	1:A:348:ARG:NH1	2.26	0.51
1:D:234:VAL:C	1:D:236:LYS:N	2.67	0.51
1:E:134:GLU:OE2	1:E:229:GLY:HA2	2.10	0.51
1:F:200:ILE:HD11	1:F:230:THR:CG2	2.41	0.51
1:E:234:VAL:HG21	1:E:236:LYS:CG	2.40	0.51
1:A:36:ARG:HH12	1:A:38:ALA:HB2	1.76	0.51
1:E:91:ARG:HG2	1:E:92:ALA:N	2.22	0.51
1:E:186:LEU:HD21	1:E:261:PHE:HB2	1.93	0.51
1:F:59:PHE:HB2	1:F:129:LEU:HD12	1.92	0.51
1:D:161:LEU:O	1:D:162:PRO:C	2.54	0.51
1:D:366:ARG:HD3	1:D:389:THR:HG21	1.91	0.51
1:A:358:THR:C	1:A:360:GLY:H	2.19	0.50
1:A:33:LEU:HD11	1:A:60:ASP:CB	2.42	0.50
1:B:312:ALA:O	1:B:313:ASP:C	2.54	0.50
1:D:36:ARG:N	1:D:37:PRO:CD	2.75	0.50
1:F:364:LEU:HD21	1:F:366:ARG:NH2	2.26	0.50
1:A:168:ARG:NH1	1:A:203:ALA:HB1	2.27	0.50
1:D:28:TRP:HE1	1:D:219:ILE:HG22	1.76	0.50
1:D:269:HIS:HB3	1:D:356:PHE:O	2.10	0.50
1:A:14:THR:HB	1:A:74:VAL:HG22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:VAL:HB	1:A:191:LEU:HB3	1.92	0.50
1:D:139:LEU:HB3	1:D:193:TRP:CD1	2.47	0.50
1:F:16:ARG:CD	1:F:97:PRO:HB2	2.42	0.50
1:D:19:ARG:NH2	1:D:91:ARG:HA	2.23	0.50
1:F:22:PHE:O	1:F:26:VAL:HG23	2.12	0.50
1:A:169:VAL:HG12	1:A:178:LEU:HD22	1.93	0.50
1:C:347:LEU:HB3	1:C:367:PRO:HB3	1.93	0.49
1:E:359:ALA:HB3	1:E:399:ARG:HH21	1.76	0.49
1:B:372:ASP:O	1:B:374:PRO:HD3	2.13	0.49
1:A:59:PHE:CB	1:A:64:SER:HA	2.35	0.49
1:D:259:PRO:HB3	1:F:163:MET:HG2	1.94	0.49
1:E:206:VAL:CG2	1:E:207:PRO:HD2	2.31	0.49
1:A:274:THR:HA	1:A:352:VAL:O	2.12	0.49
1:A:357:THR:HG22	1:A:358:THR:HG23	1.95	0.49
1:F:396:MET:HE3	1:F:397:PRO:HD2	1.94	0.49
1:A:36:ARG:NH1	1:A:38:ALA:CB	2.73	0.49
1:A:290:VAL:HG12	1:A:290:VAL:O	2.12	0.49
1:E:314:ASP:O	1:E:315:VAL:HG12	2.13	0.49
1:A:151:VAL:CG2	1:A:167:ILE:HD13	2.42	0.49
1:D:163:MET:HE3	1:D:257:GLU:C	2.36	0.49
1:E:20:GLU:CD	1:E:20:GLU:N	2.60	0.49
1:F:41:VAL:HG21	1:F:125:ASP:HB3	1.95	0.49
1:A:33:LEU:HD21	1:A:60:ASP:OD1	2.12	0.49
1:D:228:LEU:O	1:D:235:GLY:HA2	2.13	0.49
1:F:63:VAL:HB	1:F:251:THR:HA	1.95	0.49
1:B:284:ILE:HD13	1:B:308:LEU:HD21	1.94	0.48
1:C:297:VAL:HG23	1:C:337:PRO:HG3	1.93	0.48
1:E:150:GLN:OE1	1:E:189:ARG:HD3	2.12	0.48
1:F:22:PHE:CD2	1:F:98:VAL:HG21	2.46	0.48
1:D:129:LEU:HD22	1:D:129:LEU:N	2.27	0.48
1:F:275:MET:HE1	1:F:306:VAL:HG11	1.95	0.48
1:A:114:ALA:CB	1:B:320:GLU:HG2	2.43	0.48
1:C:96:LYS:HD2	1:C:112:GLY:HA3	1.94	0.48
1:D:109:LEU:HB3	1:D:116:PHE:HB2	1.95	0.48
1:E:289:LEU:HD23	1:F:89:ILE:HA	1.95	0.48
1:F:59:PHE:HB2	1:F:129:LEU:CD1	2.43	0.48
1:C:296:GLN:HG3	1:C:334:ALA:HB1	1.96	0.48
1:D:48:THR:HG23	1:D:78:SER:HB3	1.94	0.48
1:E:15:PHE:CD2	1:E:17:LEU:HD13	2.48	0.48
1:E:32:ASN:CG	1:E:32:ASN:O	2.56	0.48
1:A:315:VAL:HA	1:B:119:PRO:CG	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:THR:O	1:B:181:THR:HG23	2.12	0.48
1:E:35:ALA:HB1	1:E:39:VAL:HG23	1.94	0.48
1:D:296:GLN:HG2	1:D:398:VAL:HG21	1.94	0.48
1:A:166:GLY:HA2	1:A:207:PRO:HA	1.96	0.48
1:E:236:LYS:O	1:E:237:ASP:HB2	2.13	0.48
1:E:365:LEU:HD23	1:E:365:LEU:N	2.28	0.48
1:F:262:ARG:HA	1:F:265:LEU:HD12	1.95	0.48
1:F:232:PRO:HG2	1:F:233:GLY:H	1.79	0.48
1:A:157:ARG:O	1:A:157:ARG:CD	2.57	0.47
1:C:13:LEU:HD13	1:C:77:GLY:O	2.14	0.47
1:E:206:VAL:HG23	1:E:207:PRO:CD	2.31	0.47
1:E:238:GLY:C	1:E:253:LEU:HD22	2.39	0.47
1:C:340:LEU:O	1:C:344:LEU:HD22	2.15	0.47
1:D:80:LEU:HD23	1:D:121:MET:HB2	1.94	0.47
1:F:59:PHE:CE2	1:F:130:PRO:HD3	2.48	0.47
1:E:167:ILE:HG13	1:E:208:ALA:HA	1.96	0.47
1:A:90:THR:HA	1:A:93:LEU:HD12	1.97	0.47
1:A:161:LEU:N	1:A:161:LEU:CD1	2.61	0.47
1:C:98:VAL:HB	1:C:111:CYS:HB2	1.97	0.47
1:B:146:GLU:HG3	1:B:348:ARG:HH11	1.79	0.47
1:C:298:ARG:HD2	1:C:309:SER:OG	2.15	0.47
1:E:204:VAL:HG21	1:E:253:LEU:HG	1.94	0.47
1:F:34:PRO:HB2	1:F:36:ARG:CZ	2.44	0.47
1:F:37:PRO:CG	1:F:43:SER:HB3	2.35	0.47
1:F:148:ILE:HD12	1:F:211:LEU:HD13	1.95	0.47
1:F:298:ARG:HH22	1:F:311:GLY:N	2.12	0.47
1:A:233:GLY:O	1:A:234:VAL:HG22	2.14	0.47
1:A:236:LYS:HD2	1:A:236:LYS:O	2.14	0.47
1:E:168:ARG:NH1	1:E:203:ALA:HB1	2.29	0.47
1:C:271:ALA:HB3	1:C:356:PHE:HB2	1.97	0.47
1:C:307:ARG:HG3	1:C:321:ASP:OD2	2.14	0.47
1:A:205:LEU:HD23	1:A:254:LEU:HD13	1.96	0.47
1:B:306:VAL:HG12	1:B:324:VAL:HB	1.96	0.47
1:B:354:PHE:CE1	1:B:365:LEU:HD22	2.50	0.47
1:E:206:VAL:HB	1:E:253:LEU:CD1	2.45	0.47
1:A:181:THR:HG22	1:A:258:PHE:HZ	1.78	0.46
1:A:387:VAL:CG2	1:A:388:SER:N	2.73	0.46
1:F:270:THR:HG23	1:F:357:THR:HG23	1.97	0.46
1:E:358:THR:C	1:E:360:GLY:H	2.24	0.46
1:A:399:ARG:H	1:A:399:ARG:CD	2.28	0.46
1:D:148:ILE:CG2	1:D:212:ALA:HA	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:13:LEU:O	1:E:102:VAL:CG1	2.64	0.46
1:A:93:LEU:HD22	1:A:111:CYS:HB3	1.97	0.46
1:B:106:ARG:NH2	1:B:117:SER:O	2.48	0.46
1:D:234:VAL:O	1:D:235:GLY:C	2.59	0.46
1:D:273:ALA:HB2	1:D:326:TYR:HD1	1.80	0.46
1:E:334:ALA:HB3	1:E:398:VAL:O	2.15	0.46
1:B:275:MET:HE2	1:B:280:LEU:HD13	1.97	0.46
1:E:221:GLY:C	1:E:223:ASP:H	2.24	0.46
1:F:296:GLN:CB	1:F:337:PRO:HD3	2.27	0.46
1:A:135:GLU:OE2	1:A:138:LEU:HD12	2.15	0.46
1:A:356:PHE:CD2	1:A:356:PHE:N	2.80	0.46
1:E:315:VAL:O	1:F:106:ARG:NH2	2.45	0.46
1:F:200:ILE:HD11	1:F:230:THR:HG22	1.97	0.46
1:A:98:VAL:HG12	1:A:111:CYS:SG	2.55	0.46
1:B:296:GLN:HA	1:B:337:PRO:HD3	1.96	0.46
1:E:15:PHE:CE2	1:E:17:LEU:HD13	2.50	0.46
1:E:245:ASN:C	1:E:247:LYS:H	2.24	0.46
1:F:14:THR:OG1	1:F:101:HIS:HD2	1.99	0.46
1:C:288:ALA:C	1:C:290:VAL:H	2.24	0.46
1:F:100:VAL:HA	1:F:108:ALA:O	2.16	0.46
1:F:42:LEU:CD1	1:F:59:PHE:O	2.64	0.46
1:A:298:ARG:HH22	1:A:400:LEU:HA	1.81	0.45
1:D:143:LEU:HD22	1:D:191:LEU:HD21	1.98	0.45
1:D:236:LYS:HD2	1:D:236:LYS:HA	1.68	0.45
1:D:275:MET:HE1	1:D:306:VAL:HG11	1.97	0.45
1:E:134:GLU:CD	1:E:229:GLY:HA2	2.41	0.45
1:E:164:LEU:C	1:E:166:GLY:H	2.23	0.45
1:E:313:ASP:C	1:E:315:VAL:H	2.24	0.45
1:A:254:LEU:H	1:A:254:LEU:HD12	1.82	0.45
1:B:384:PHE:N	1:B:385:PRO:CD	2.79	0.45
1:D:217:ALA:O	1:D:219:ILE:HG23	2.16	0.45
1:F:51:ASP:C	1:F:53:GLY:N	2.74	0.45
1:F:164:LEU:HD21	1:F:182:ASP:HA	1.98	0.45
1:C:291:ALA:HA	1:C:311:GLY:O	2.17	0.45
1:A:198:PRO:O	1:A:199:ASP:C	2.59	0.45
1:B:170:GLU:OE1	1:B:262:ARG:NH2	2.50	0.45
1:E:79:VAL:HG21	1:E:107:VAL:HG21	1.99	0.45
1:A:149:SER:HB2	1:A:216:LYS:NZ	2.31	0.45
1:A:364:LEU:HD12	1:A:366:ARG:HG3	1.99	0.45
1:D:259:PRO:HG2	1:F:163:MET:HE3	1.99	0.45
1:F:304:GLY:HA2	1:F:324:VAL:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45:VAL:HG23	1:C:57:SER:O	2.16	0.45
1:D:155:ALA:O	1:D:156:GLY:O	2.35	0.45
1:E:24:ASP:C	1:E:24:ASP:OD1	2.59	0.45
1:E:161:LEU:CD2	1:E:163:MET:HE1	2.47	0.45
1:F:74:VAL:HG12	1:F:75:SER:OG	2.16	0.45
1:D:148:ILE:HG21	1:D:212:ALA:HA	1.99	0.45
1:D:170:GLU:OE1	1:D:262:ARG:NH2	2.50	0.45
1:D:219:ILE:O	1:D:219:ILE:CG1	2.65	0.45
1:A:364:LEU:CD2	1:A:394:LEU:HD12	2.46	0.45
1:B:78:SER:OG	1:B:123:VAL:HG11	2.17	0.45
1:C:146:GLU:O	1:C:150:GLN:HG3	2.16	0.45
1:C:284:ILE:C	1:C:286:LEU:H	2.24	0.45
1:D:185:ARG:NH2	1:D:342:ASP:OD2	2.50	0.45
1:B:50:SER:HB3	1:B:51:ASP:H	1.64	0.44
1:C:206:VAL:HG21	1:C:211:LEU:HG	1.99	0.44
1:E:204:VAL:HG22	1:E:205:LEU:N	2.33	0.44
1:A:269:HIS:CD2	1:A:272:VAL:HG12	2.51	0.44
1:D:137:GLY:HA3	1:D:193:TRP:CH2	2.52	0.44
1:D:299:MET:HE2	1:D:335:PHE:CE2	2.53	0.44
1:E:15:PHE:CE2	1:E:17:LEU:CD1	3.00	0.44
1:F:299:MET:HE2	1:F:335:PHE:CE2	2.52	0.44
1:A:357:THR:CG2	1:A:361:LYS:HD2	2.48	0.44
1:C:315:VAL:HG13	1:D:106:ARG:HH22	1.81	0.44
1:D:159:ASP:C	1:D:161:LEU:N	2.75	0.44
1:E:186:LEU:HB3	1:E:394:LEU:HB3	1.99	0.44
1:A:283:ALA:HA	1:A:286:LEU:HB2	2.00	0.44
1:A:293:ARG:HA	1:A:293:ARG:HD2	1.81	0.44
1:C:134:GLU:CD	1:C:134:GLU:H	2.23	0.44
1:C:182:ASP:C	1:C:184:PHE:H	2.26	0.44
1:A:148:ILE:H	1:A:148:ILE:HG12	1.47	0.44
1:A:167:ILE:HG12	1:A:180:ALA:HB2	1.99	0.44
1:E:17:LEU:HB3	1:E:71:ALA:HB1	2.00	0.44
1:F:280:LEU:HG	1:F:284:ILE:HD11	1.99	0.44
1:A:106:ARG:CG	1:A:106:ARG:NH1	2.78	0.44
1:A:152:ALA:HB2	1:A:167:ILE:HD11	2.00	0.44
1:C:171:ILE:HG21	1:C:193:TRP:HZ3	1.83	0.44
1:E:237:ASP:N	1:E:237:ASP:OD1	2.51	0.44
1:F:231:GLY:O	1:F:232:PRO:C	2.61	0.44
1:F:273:ALA:HB2	1:F:326:TYR:HD1	1.83	0.44
1:D:217:ALA:O	1:D:219:ILE:N	2.50	0.44
1:E:292:ASP:O	1:E:293:ARG:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:133:PRO:HG2	1:F:227:SER:O	2.17	0.44
1:C:301:PHE:HB3	1:C:326:TYR:CE1	2.53	0.44
1:D:366:ARG:HD2	1:D:389:THR:CG2	2.41	0.44
1:F:60:ASP:HB3	1:F:63:VAL:O	2.18	0.44
1:A:182:ASP:OD1	1:A:183:ARG:N	2.49	0.44
1:A:273:ALA:HB2	1:A:326:TYR:CD1	2.44	0.44
1:B:60:ASP:HB3	1:B:63:VAL:O	2.18	0.44
1:B:335:PHE:CD1	1:B:395:LEU:HD13	2.53	0.44
1:E:63:VAL:HG23	1:E:250:THR:O	2.18	0.44
1:F:64:SER:O	1:F:249:SER:HB2	2.18	0.44
1:F:350:GLU:HG2	1:F:351:ARG:HG2	2.00	0.44
1:A:45:VAL:HG23	1:A:57:SER:O	2.18	0.43
1:B:33:LEU:HA	1:B:34:PRO:HD3	1.87	0.43
1:B:167:ILE:HG13	1:B:208:ALA:HB2	2.00	0.43
1:C:204:VAL:HG22	1:C:253:LEU:HG	2.00	0.43
1:E:236:LYS:O	1:E:237:ASP:CB	2.65	0.43
1:A:146:GLU:HG3	1:A:348:ARG:HH12	1.81	0.43
1:F:80:LEU:HD23	1:F:121:MET:CB	2.39	0.43
1:F:219:ILE:O	1:F:219:ILE:HG12	2.18	0.43
1:A:188:VAL:HB	1:A:392:VAL:HG12	1.99	0.43
1:E:131:THR:CA	1:E:133:PRO:HD3	2.48	0.43
1:F:59:PHE:HD2	1:F:129:LEU:HA	1.83	0.43
1:A:171:ILE:HG12	1:A:193:TRP:CZ3	2.54	0.43
1:A:234:VAL:O	1:A:237:ASP:OD1	2.35	0.43
1:C:99:ASP:OD2	1:C:99:ASP:N	2.51	0.43
1:B:290:VAL:HG13	1:B:290:VAL:O	2.19	0.43
1:F:25:ALA:CB	1:F:56:ILE:HD12	2.43	0.43
1:F:290:VAL:HG21	1:F:318:ALA:N	2.34	0.43
1:A:35:ALA:CA	1:A:84:ARG:HE	2.18	0.43
1:A:362:PRO:HG3	1:A:396:MET:SD	2.58	0.43
1:D:161:LEU:HD22	1:F:183:ARG:HD3	2.00	0.43
1:D:239:LEU:HD23	1:D:250:THR:HB	2.01	0.43
1:A:185:ARG:NH1	1:A:342:ASP:OD2	2.45	0.43
1:A:148:ILE:HG23	1:A:148:ILE:HD13	1.57	0.43
1:B:226:LEU:HD12	1:B:242:ILE:HG22	2.01	0.43
1:C:55:THR:HA	1:C:67:ALA:O	2.18	0.43
1:C:270:THR:HG23	1:C:357:THR:HA	2.00	0.43
1:F:300:GLU:HG3	1:F:332:THR:HG23	2.00	0.43
1:B:192:LYS:H	1:B:192:LYS:CD	2.31	0.43
1:C:262:ARG:HE	1:C:262:ARG:HB2	1.69	0.43
1:D:231:GLY:O	1:D:232:PRO:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:ALA:O	1:A:209:LYS:C	2.62	0.43
1:A:399:ARG:HG2	1:A:400:LEU:H	1.83	0.43
1:D:261:PHE:HA	1:D:264:LEU:HD12	2.00	0.43
1:D:274:THR:HA	1:D:352:VAL:O	2.18	0.43
1:D:396:MET:HE2	1:F:158:ASP:O	2.19	0.43
1:E:29:VAL:C	1:E:31:LYS:H	2.26	0.43
1:F:36:ARG:C	1:F:36:ARG:CD	2.91	0.43
1:A:173:GLY:HA2	1:A:199:ASP:HA	2.00	0.42
1:C:29:VAL:HG13	1:C:58:GLY:HA3	2.01	0.42
1:E:302:ALA:O	1:E:303:ASP:C	2.61	0.42
1:F:16:ARG:NE	1:F:99:ASP:OD2	2.52	0.42
1:F:222:SER:OG	1:F:223:ASP:N	2.50	0.42
1:F:364:LEU:HD13	1:F:394:LEU:HD23	2.00	0.42
1:B:80:LEU:HB2	1:B:123:VAL:HG22	2.01	0.42
1:E:28:TRP:CH2	1:E:247:LYS:HB3	2.54	0.42
1:E:132:LEU:HB2	1:E:239:LEU:HD22	2.02	0.42
1:B:46:LEU:HB3	1:B:57:SER:HB2	2.01	0.42
1:F:42:LEU:HD11	1:F:59:PHE:O	2.18	0.42
1:B:54:LEU:HD13	1:B:54:LEU:O	2.19	0.42
1:B:189:ARG:HA	1:B:189:ARG:HD2	1.87	0.42
1:B:353:SER:O	1:B:365:LEU:HA	2.19	0.42
1:C:91:ARG:HB3	1:C:91:ARG:NH1	2.33	0.42
1:D:42:LEU:HG	1:D:60:ASP:HA	2.02	0.42
1:A:312:ALA:C	1:A:314:ASP:H	2.28	0.42
1:C:290:VAL:HG12	1:C:290:VAL:O	2.20	0.42
1:E:171:ILE:HG23	1:E:193:TRP:HZ3	1.84	0.42
1:E:185:ARG:NH2	1:E:339:TYR:HD1	2.17	0.42
1:B:45:VAL:HG13	1:B:47:LEU:HD13	2.01	0.42
1:B:354:PHE:CD1	1:B:356:PHE:HZ	2.34	0.42
1:A:262:ARG:HA	1:A:265:LEU:HD12	2.01	0.42
1:A:281:ILE:HD11	1:A:344:LEU:HB3	2.00	0.42
1:B:14:THR:HA	1:B:100:VAL:O	2.20	0.42
1:C:92:ALA:O	1:D:286:LEU:HD13	2.20	0.42
1:F:59:PHE:HE2	1:F:130:PRO:HD3	1.84	0.42
1:F:139:LEU:HB3	1:F:193:TRP:CD1	2.54	0.42
1:A:48:THR:HB	1:A:55:THR:OG1	2.20	0.42
1:E:350:GLU:HB3	1:E:351:ARG:HG2	2.01	0.42
1:F:336:ASN:OD1	1:F:336:ASN:C	2.62	0.42
1:C:353:SER:HB3	1:C:366:ARG:HG3	2.00	0.42
1:D:232:PRO:HG2	1:D:233:GLY:H	1.84	0.42
1:D:357:THR:HG22	1:D:358:THR:HG23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:161:LEU:HA	1:F:162:PRO:HD3	1.81	0.42
1:F:366:ARG:HB3	1:F:389:THR:HG21	2.01	0.42
1:B:368:VAL:O	1:B:370:GLY:N	2.47	0.42
1:D:28:TRP:HE1	1:D:219:ILE:CG2	2.33	0.42
1:E:85:LEU:HD22	1:F:315:VAL:HG22	2.02	0.42
1:E:206:VAL:HB	1:E:253:LEU:HD12	2.02	0.42
1:A:40:PRO:O	1:A:42:LEU:N	2.52	0.41
1:B:300:GLU:HB2	1:B:307:ARG:HB3	2.02	0.41
1:C:239:LEU:HG	1:C:250:THR:HB	2.01	0.41
1:C:358:THR:HG23	1:C:361:LYS:HE3	2.02	0.41
1:F:290:VAL:HG21	1:F:317:ARG:C	2.45	0.41
1:F:357:THR:HB	1:F:361:LYS:HE3	2.02	0.41
1:C:75:SER:HA	1:C:76:PRO:HD3	1.91	0.41
1:E:135:GLU:H	1:E:135:GLU:HG3	1.58	0.41
1:B:99:ASP:HB2	1:B:110:THR:HB	2.02	0.41
1:B:147:ALA:HB1	1:B:178:LEU:HD12	2.01	0.41
1:D:47:LEU:O	1:D:78:SER:HA	2.20	0.41
1:E:319:GLU:HB2	1:F:115:ARG:HB2	2.03	0.41
1:A:93:LEU:HA	1:B:286:LEU:HD11	2.01	0.41
1:C:59:PHE:HB2	1:C:129:LEU:CD2	2.50	0.41
1:C:346:SER:O	1:C:348:ARG:HD2	2.20	0.41
1:E:37:PRO:HB2	1:E:38:ALA:H	1.62	0.41
1:E:161:LEU:HD22	1:E:163:MET:HE1	2.03	0.41
1:F:163:MET:HE2	1:F:183:ARG:NH1	2.35	0.41
1:F:268:GLU:HG3	1:F:269:HIS:H	1.85	0.41
1:B:153:ILE:HD11	1:B:346:SER:HB2	2.01	0.41
1:D:150:GLN:HE21	1:D:348:ARG:HD2	1.86	0.41
1:E:290:VAL:HG11	1:E:316:GLY:O	2.19	0.41
1:F:98:VAL:HA	1:F:111:CYS:SG	2.61	0.41
1:A:40:PRO:C	1:A:42:LEU:N	2.78	0.41
1:A:146:GLU:O	1:A:147:ALA:C	2.64	0.41
1:B:386:ALA:O	1:B:387:VAL:CG1	2.68	0.41
1:C:41:VAL:HG11	1:C:125:ASP:HB3	2.03	0.41
1:D:59:PHE:CD1	1:D:64:SER:HB2	2.55	0.41
1:E:15:PHE:HE2	1:E:17:LEU:HD11	1.84	0.41
1:E:79:VAL:CG2	1:E:80:LEU:N	2.84	0.41
1:F:218:GLY:CA	1:F:245:ASN:ND2	2.79	0.41
1:A:33:LEU:CD2	1:A:63:VAL:HG13	2.51	0.41
1:A:169:VAL:HG23	1:A:204:VAL:HG12	2.03	0.41
1:C:93:LEU:HD11	1:C:109:LEU:HD11	2.02	0.41
1:D:162:PRO:O	1:D:163:MET:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:268:GLU:HG3	1:F:269:HIS:N	2.35	0.41
1:A:52:ASN:C	1:A:73:ILE:HD11	2.45	0.41
1:A:152:ALA:O	1:A:157:ARG:NH2	2.54	0.41
1:A:269:HIS:HD2	1:A:272:VAL:HG13	1.85	0.41
1:B:100:VAL:HA	1:B:108:ALA:O	2.21	0.41
1:B:274:THR:HA	1:B:352:VAL:O	2.21	0.41
1:C:93:LEU:HD23	1:D:286:LEU:HD21	2.03	0.41
1:C:275:MET:HB3	1:C:324:VAL:HG12	2.03	0.41
1:C:294:GLY:O	1:C:337:PRO:HD2	2.21	0.41
1:D:152:ALA:HB2	1:D:167:ILE:HD11	2.03	0.41
1:E:79:VAL:HG22	1:E:80:LEU:N	2.35	0.41
1:E:106:ARG:CG	1:E:106:ARG:NH1	2.83	0.41
1:E:299:MET:HG2	1:E:308:LEU:HD12	2.02	0.41
1:F:59:PHE:CD2	1:F:129:LEU:HA	2.56	0.41
1:F:126:TYR:HA	1:F:127:PRO:HD3	1.94	0.41
1:A:195:ALA:C	1:A:197:SER:H	2.29	0.41
1:C:33:LEU:HD11	1:C:45:VAL:HB	2.03	0.41
1:D:29:VAL:C	1:D:31:LYS:H	2.29	0.41
1:D:255:ASP:OD2	1:D:255:ASP:N	2.54	0.41
1:D:297:VAL:HG13	1:D:337:PRO:HG3	2.02	0.41
1:E:205:LEU:HD23	1:E:254:LEU:HB2	2.03	0.41
1:A:42:LEU:HD11	1:A:60:ASP:HA	2.03	0.40
1:A:314:ASP:CG	1:A:315:VAL:HG23	2.46	0.40
1:B:54:LEU:HD12	1:B:69:VAL:CG1	2.50	0.40
1:B:197:SER:HB2	1:B:200:ILE:HD13	2.02	0.40
1:C:134:GLU:OE1	1:C:229:GLY:HA2	2.21	0.40
1:E:29:VAL:C	1:E:31:LYS:N	2.79	0.40
1:E:287:VAL:O	1:E:310:ALA:HB3	2.21	0.40
1:F:299:MET:HE2	1:F:335:PHE:HE2	1.86	0.40
1:A:336:ASN:OD1	1:A:336:ASN:C	2.64	0.40
1:A:228:LEU:O	1:A:234:VAL:HB	2.21	0.40
1:B:154:ALA:O	1:B:155:ALA:C	2.65	0.40
1:C:283:ALA:O	1:C:287:VAL:HG22	2.22	0.40
1:C:286:LEU:HG	1:D:116:PHE:HZ	1.86	0.40
1:B:44:GLY:HA2	1:B:83:GLY:H	1.87	0.40
1:E:274:THR:OG1	1:E:325:ASP:HB2	2.21	0.40
1:A:14:THR:HA	1:A:100:VAL:O	2.21	0.40
1:A:157:ARG:HB3	1:A:165:THR:HG21	2.03	0.40
1:A:299:MET:HE2	1:A:335:PHE:CD2	2.56	0.40
1:C:232:PRO:O	1:C:234:VAL:HG12	2.22	0.40
1:D:14:THR:HG23	1:D:101:HIS:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:162:PRO:HA	1:E:165:THR:OG1	2.21	0.40
1:E:296:GLN:NE2	1:E:400:LEU:HD22	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	B	170/322 (53%)	133 (78%)	37 (22%)	1	3
1	C	294/322 (91%)	229 (78%)	65 (22%)	1	3
1	D	293/322 (91%)	231 (79%)	62 (21%)	1	4
1	E	293/322 (91%)	228 (78%)	65 (22%)	1	3
1	F	295/322 (92%)	231 (78%)	64 (22%)	1	3
All	All	1345/1610 (84%)	1052 (78%)	293 (22%)	1	3

All (293) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	183	ARG
1	B	185	ARG
1	B	186	LEU
1	B	191	LEU
1	B	192	LYS
1	B	196	SER
1	B	204	VAL

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Mol	Chain	Res	Type
1	B	206	VAL
1	B	209	LYS
1	B	211	LEU
1	B	219	ILE
1	B	226	LEU
1	B	236	LYS
1	B	242	ILE
1	B	245	ASN
1	B	251	THR
1	B	252	ARG
1	B	253	LEU
1	B	254	LEU
1	B	263	GLN
1	B	285	LYS
1	B	286	LEU
1	B	289	LEU
1	B	290	VAL
1	B	300	GLU
1	B	313	ASP
1	B	317	ARG
1	B	329	GLU
1	B	341	THR
1	B	344	LEU
1	B	347	LEU
1	B	365	LEU
1	B	371	ASP
1	B	378	LEU
1	B	389	THR
1	B	395	LEU
1	B	400	LEU
1	C	18	LEU
1	C	48	THR
1	C	54	LEU
1	C	56	ILE
1	C	63	VAL
1	C	74	VAL
1	C	85	LEU
1	C	91	ARG
1	C	98	VAL
1	C	99	ASP
1	C	105	ASN
1	C	109	LEU

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Mol	Chain	Res	Type
1	C	113	ASN
1	C	115	ARG
1	C	120	THR
1	C	124	GLU
1	C	125	ASP
1	C	128	THR
1	C	131	THR
1	C	134	GLU
1	C	138	LEU
1	C	139	LEU
1	C	142	GLU
1	C	143	LEU
1	C	148	ILE
1	C	153	ILE
1	C	160	THR
1	C	161	LEU
1	C	163	MET
1	C	185	ARG
1	C	191	LEU
1	C	192	LYS
1	C	204	VAL
1	C	206	VAL
1	C	210	THR
1	C	211	LEU
1	C	213	GLU
1	C	219	ILE
1	C	234	VAL
1	C	236	LYS
1	C	245	ASN
1	C	247	LYS
1	C	253	LEU
1	C	262	ARG
1	C	267	THR
1	C	279	GLU
1	C	289	LEU
1	C	293	ARG
1	C	297	VAL
1	C	298	ARG
1	C	309	SER
1	C	314	ASP
1	C	320	GLU
1	C	341	THR

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Mol	Chain	Res	Type
1	C	344	LEU
1	C	346	SER
1	C	347	LEU
1	C	352	VAL
1	C	358	THR
1	C	365	LEU
1	C	368	VAL
1	C	388	SER
1	C	394	LEU
1	C	395	LEU
1	C	400	LEU
1	D	21	SER
1	D	33	LEU
1	D	36	ARG
1	D	41	VAL
1	D	42	LEU
1	D	45	VAL
1	D	48	THR
1	D	50	SER
1	D	51	ASP
1	D	52	ASN
1	D	54	LEU
1	D	69	VAL
1	D	73	ILE
1	D	75	SER
1	D	79	VAL
1	D	85	LEU
1	D	105	ASN
1	D	109	LEU
1	D	110	THR
1	D	120	THR
1	D	128	THR
1	D	129	LEU
1	D	131	THR
1	D	134	GLU
1	D	138	LEU
1	D	142	GLU
1	D	143	LEU
1	D	158	ASP
1	D	172	LEU
1	D	174	GLU
1	D	185	ARG

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Mol	Chain	Res	Type
1	D	191	LEU
1	D	192	LYS
1	D	196	SER
1	D	204	VAL
1	D	206	VAL
1	D	211	LEU
1	D	219	ILE
1	D	226	LEU
1	D	230	THR
1	D	236	LYS
1	D	237	ASP
1	D	239	LEU
1	D	242	ILE
1	D	245	ASN
1	D	253	LEU
1	D	255	ASP
1	D	270	THR
1	D	272	VAL
1	D	282	GLU
1	D	308	LEU
1	D	313	ASP
1	D	320	GLU
1	D	329	GLU
1	D	341	THR
1	D	344	LEU
1	D	346	SER
1	D	347	LEU
1	D	369	SER
1	D	389	THR
1	D	395	LEU
1	D	399	ARG
1	E	13	LEU
1	E	17	LEU
1	E	18	LEU
1	E	21	SER
1	E	24	ASP
1	E	32	ASN
1	E	45	VAL
1	E	48	THR
1	E	52	ASN
1	E	54	LEU
1	E	63	VAL

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Mol	Chain	Res	Type
1	E	72	GLU
1	E	73	ILE
1	E	79	VAL
1	E	91	ARG
1	E	93	LEU
1	E	95	ASN
1	E	96	LYS
1	E	99	ASP
1	E	102	VAL
1	E	105	ASN
1	E	106	ARG
1	E	107	VAL
1	E	115	ARG
1	E	123	VAL
1	E	129	LEU
1	E	131	THR
1	E	135	GLU
1	E	139	LEU
1	E	143	LEU
1	E	151	VAL
1	E	158	ASP
1	E	163	MET
1	E	183	ARG
1	E	185	ARG
1	E	191	LEU
1	E	192	LYS
1	E	206	VAL
1	E	209	LYS
1	E	210	THR
1	E	211	LEU
1	E	237	ASP
1	E	239	LEU
1	E	240	LEU
1	E	242	ILE
1	E	243	SER
1	E	250	THR
1	E	253	LEU
1	E	263	GLN
1	E	272	VAL
1	E	286	LEU
1	E	289	LEU
1	E	290	VAL

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Mol	Chain	Res	Type
1	E	296	GLN
1	E	303	ASP
1	E	309	SER
1	E	320	GLU
1	E	329	GLU
1	E	344	LEU
1	E	347	LEU
1	E	352	VAL
1	E	358	THR
1	E	365	LEU
1	E	395	LEU
1	E	400	LEU
1	F	18	LEU
1	F	19	ARG
1	F	33	LEU
1	F	36	ARG
1	F	42	LEU
1	F	47	LEU
1	F	54	LEU
1	F	63	VAL
1	F	73	ILE
1	F	78	SER
1	F	82	SER
1	F	105	ASN
1	F	107	VAL
1	F	109	LEU
1	F	110	THR
1	F	111	CYS
1	F	120	THR
1	F	125	ASP
1	F	128	THR
1	F	132	LEU
1	F	134	GLU
1	F	138	LEU
1	F	143	LEU
1	F	158	ASP
1	F	160	THR
1	F	163	MET
1	F	164	LEU
1	F	172	LEU
1	F	185	ARG
1	F	191	LEU

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Mol	Chain	Res	Type
1	F	192	LYS
1	F	199	ASP
1	F	200	ILE
1	F	204	VAL
1	F	206	VAL
1	F	209	LYS
1	F	211	LEU
1	F	219	ILE
1	F	224	VAL
1	F	226	LEU
1	F	230	THR
1	F	237	ASP
1	F	242	ILE
1	F	245	ASN
1	F	251	THR
1	F	253	LEU
1	F	262	ARG
1	F	263	GLN
1	F	264	LEU
1	F	289	LEU
1	F	297	VAL
1	F	298	ARG
1	F	314	ASP
1	F	319	GLU
1	F	320	GLU
1	F	331	LEU
1	F	344	LEU
1	F	347	LEU
1	F	351	ARG
1	F	352	VAL
1	F	357	THR
1	F	365	LEU
1	F	394	LEU
1	F	395	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	263	GLN
1	B	269	HIS
1	C	95	ASN
1	C	101	HIS

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Mol	Chain	Res	Type
1	C	245	ASN
1	D	101	HIS
1	D	245	ASN
1	D	263	GLN
1	E	32	ASN
1	E	105	ASN
1	E	263	GLN
1	F	101	HIS
1	F	105	ASN
1	F	245	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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	375/408 (91%)	0.56	19 (5%)	33	26	24, 50, 81, 95	0
1	B	383/408 (93%)	0.41	16 (4%)	40	32	17, 49, 80, 100	0
1	C	370/408 (90%)	0.48	25 (6%)	23	18	19, 46, 79, 122	0
1	D	369/408 (90%)	0.39	18 (4%)	35	27	21, 47, 79, 103	0
1	E	369/408 (90%)	0.58	21 (5%)	29	23	24, 52, 85, 118	0
1	F	372/408 (91%)	0.51	27 (7%)	21	17	19, 49, 85, 102	0
All	All	2238/2448 (91%)	0.49	126 (5%)	30	23	17, 49, 83, 122	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	295	ALA	5.6
1	F	50	SER	5.5
1	D	235	GLY	5.2
1	F	387	VAL	4.7
1	E	236	LYS	4.6
1	C	294	GLY	4.5
1	D	233	GLY	3.9
1	F	130	PRO	3.9
1	C	316	GLY	3.8
1	E	235	GLY	3.8
1	A	386	ALA	3.5
1	C	34	PRO	3.4
1	F	132	LEU	3.3
1	F	303	ASP	3.3
1	E	130	PRO	3.3
1	F	59	PHE	3.2
1	E	132	LEU	3.2
1	C	388	SER	3.2
1	E	59	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	F	131	THR	3.1
1	D	61	TYR	3.1
1	C	72	GLU	3.1
1	D	172	LEU	3.0
1	D	158	ASP	3.0
1	B	370	GLY	2.9
1	B	132	LEU	2.9
1	C	61	TYR	2.9
1	F	41	VAL	2.8
1	D	329	GLU	2.8
1	A	217	ALA	2.8
1	A	34	PRO	2.8
1	E	80	LEU	2.8
1	F	370	GLY	2.8
1	F	97	PRO	2.8
1	B	61	TYR	2.7
1	C	235	GLY	2.7
1	C	36	ARG	2.7
1	C	105	ASN	2.7
1	F	230	THR	2.7
1	C	237	ASP	2.7
1	F	237	ASP	2.7
1	F	38	ALA	2.7
1	E	61	TYR	2.7
1	A	245	ASN	2.7
1	E	388	SER	2.7
1	F	315	VAL	2.7
1	C	52	ASN	2.7
1	D	389	THR	2.7
1	F	312	ALA	2.6
1	F	316	GLY	2.6
1	C	222	SER	2.6
1	A	233	GLY	2.6
1	B	371	ASP	2.6
1	C	24	ASP	2.6
1	F	219	ILE	2.6
1	A	388	SER	2.5
1	F	400	LEU	2.5
1	C	196	SER	2.5
1	E	50	SER	2.5
1	C	133	PRO	2.5
1	E	13	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	20	GLU	2.5
1	E	76	PRO	2.5
1	C	221	GLY	2.5
1	D	193	TRP	2.5
1	D	50	SER	2.5
1	B	375	VAL	2.5
1	F	172	LEU	2.4
1	A	40	PRO	2.4
1	D	312	ALA	2.4
1	D	132	LEU	2.4
1	B	312	ALA	2.4
1	A	267	THR	2.4
1	C	313	ASP	2.3
1	A	133	PRO	2.3
1	B	198	PRO	2.3
1	F	232	PRO	2.3
1	B	221	GLY	2.3
1	B	233	GLY	2.3
1	E	233	GLY	2.3
1	B	356	PHE	2.3
1	B	196	SER	2.3
1	A	41	VAL	2.3
1	C	360	GLY	2.3
1	D	92	ALA	2.3
1	D	236	LYS	2.3
1	F	133	PRO	2.3
1	A	231	GLY	2.3
1	B	133	PRO	2.3
1	D	218	GLY	2.3
1	B	158	ASP	2.2
1	C	200	ILE	2.2
1	E	102	VAL	2.2
1	E	38	ALA	2.2
1	E	267	THR	2.2
1	E	221	GLY	2.2
1	C	73	ILE	2.2
1	D	21	SER	2.2
1	D	229	GLY	2.2
1	A	356	PHE	2.2
1	A	312	ALA	2.2
1	F	108	ALA	2.2
1	A	293	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	35	ALA	2.2
1	D	198	PRO	2.1
1	F	388	SER	2.1
1	F	314	ASP	2.1
1	A	70	GLY	2.1
1	A	35	ALA	2.1
1	A	73	ILE	2.1
1	B	13	LEU	2.1
1	C	172	LEU	2.1
1	C	400	LEU	2.1
1	D	314	ASP	2.1
1	E	93	LEU	2.1
1	E	196	SER	2.1
1	E	198	PRO	2.1
1	F	233	GLY	2.1
1	C	160	THR	2.1
1	E	73	ILE	2.1
1	A	329	GLU	2.1
1	E	94	PRO	2.0
1	B	305	SER	2.0
1	F	196	SER	2.0
1	B	59	PHE	2.0
1	A	61	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no 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.