



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:09 PM UTC

PDB ID : 4L95 / pdb_00004l95
Title : Crystal structure of gamma glutamyl hydrolase (H218N) from zebrafish
Authors : Chuankhayan, P.; Kao, T.-T.; Chen, C.-J.; Fu, T.-F.
Deposited on : 2013-06-18
Resolution : 2.34 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:

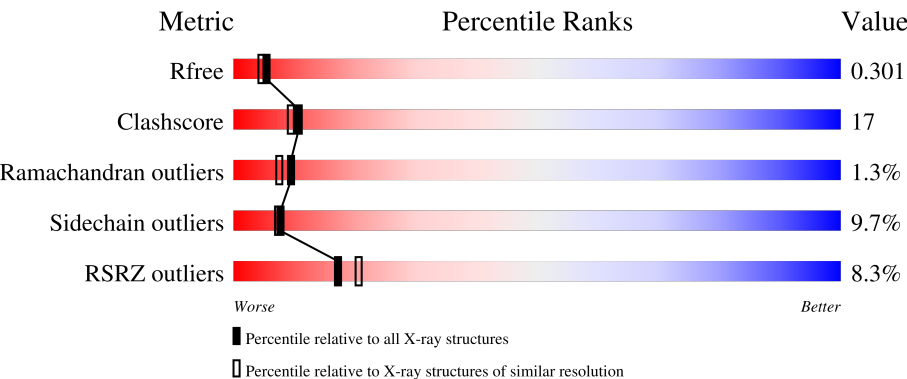
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.34 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	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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	C	312	4% 67% 20% • • 8%
1	E	312	3% 68% 20% • 8%
1	F	312	4% 67% 21% • 8%
1	G	312	4% 59% 27% 6% 8%
1	K	312	13% 51% 35% 5% • 8%

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Mol	Chain	Length	Quality of chain
1	M	312	18% 49% 36% 7% 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14068 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 Gamma-glutamyl hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	287	Total	C	N	O	S	0	0	0
			2307	1490	369	443	5			
1	F	287	Total	C	N	O	S	0	0	0
			2307	1490	369	443	5			
1	C	287	Total	C	N	O	S	0	0	0
			2307	1490	369	443	5			
1	G	287	Total	C	N	O	S	0	0	0
			2307	1490	369	443	5			
1	K	287	Total	C	N	O	S	0	0	0
			2307	1490	369	443	5			
1	M	287	Total	C	N	O	S	0	0	0
			2307	1490	369	443	5			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	218	ASN	HIS	engineered mutation	UNP Q6NY42
F	218	ASN	HIS	engineered mutation	UNP Q6NY42
C	218	ASN	HIS	engineered mutation	UNP Q6NY42
G	218	ASN	HIS	engineered mutation	UNP Q6NY42
K	218	ASN	HIS	engineered mutation	UNP Q6NY42
M	218	ASN	HIS	engineered mutation	UNP Q6NY42

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			6	3	3		
2	G	1	Total	C	O	0	0
			6	3	3		
2	K	1	Total	C	O	0	0
			6	3	3		

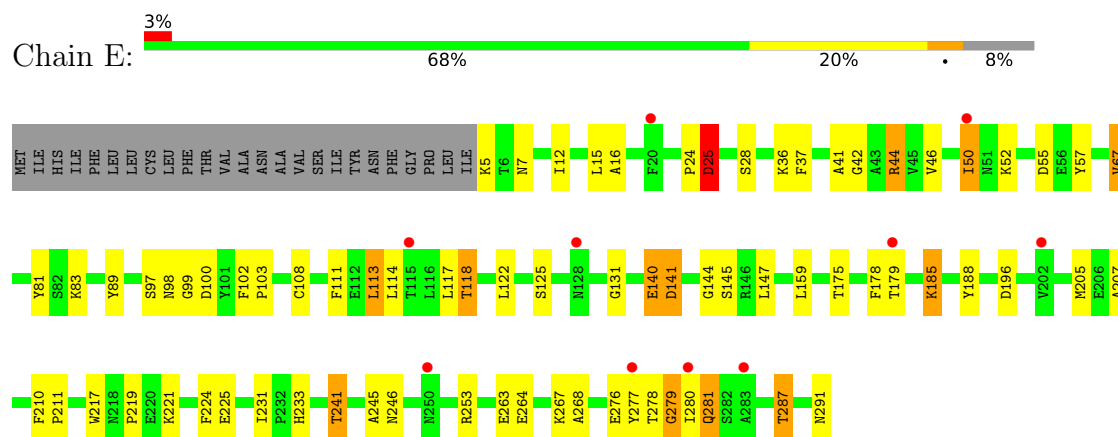
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	43	Total	O	0	0
			43	43		
3	F	39	Total	O	0	0
			39	39		
3	C	63	Total	O	0	0
			63	63		
3	G	40	Total	O	0	0
			40	40		
3	K	11	Total	O	0	0
			11	11		
3	M	12	Total	O	0	0
			12	12		

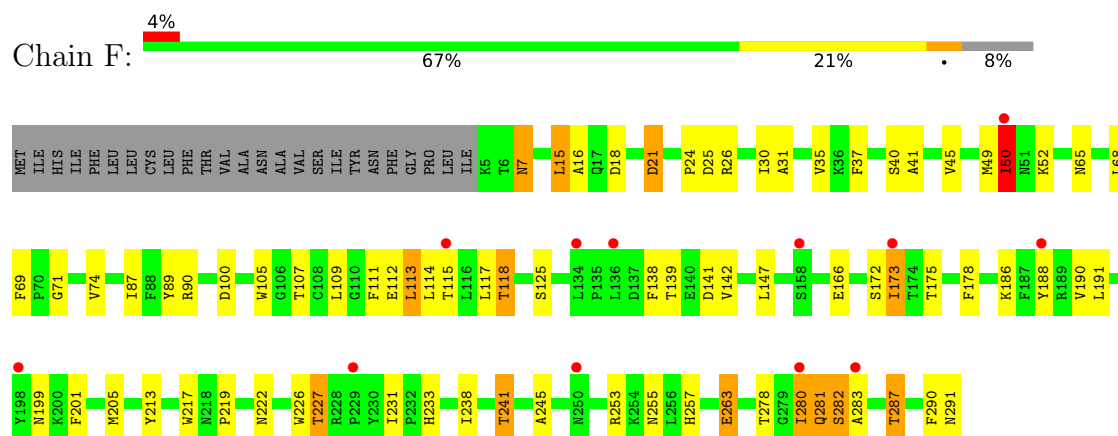
3 Residue-property plots [i](#)

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.

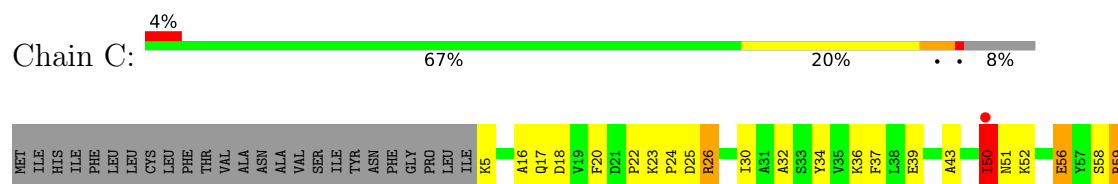
• Molecule 1: Gamma-glutamyl hydrolase

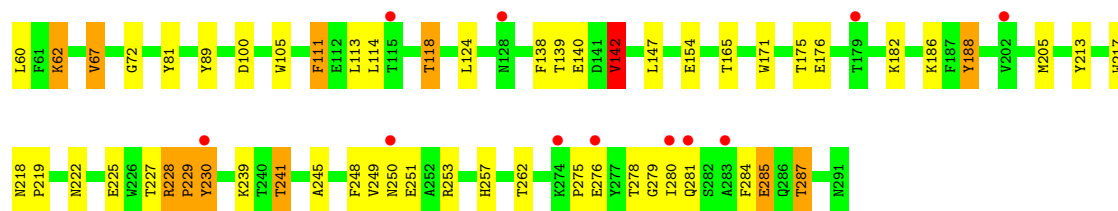


• Molecule 1: Gamma-glutamyl hydrolase

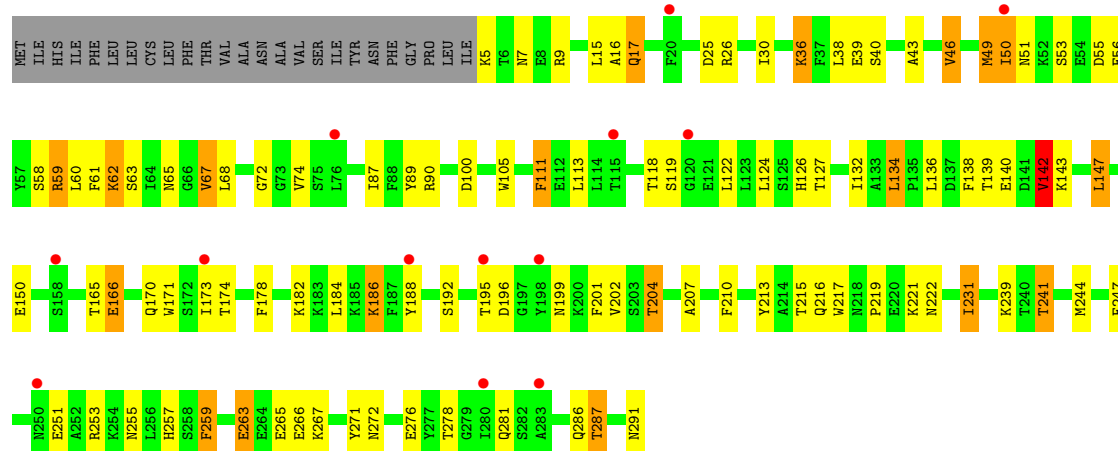


• Molecule 1: Gamma-glutamyl hydrolase

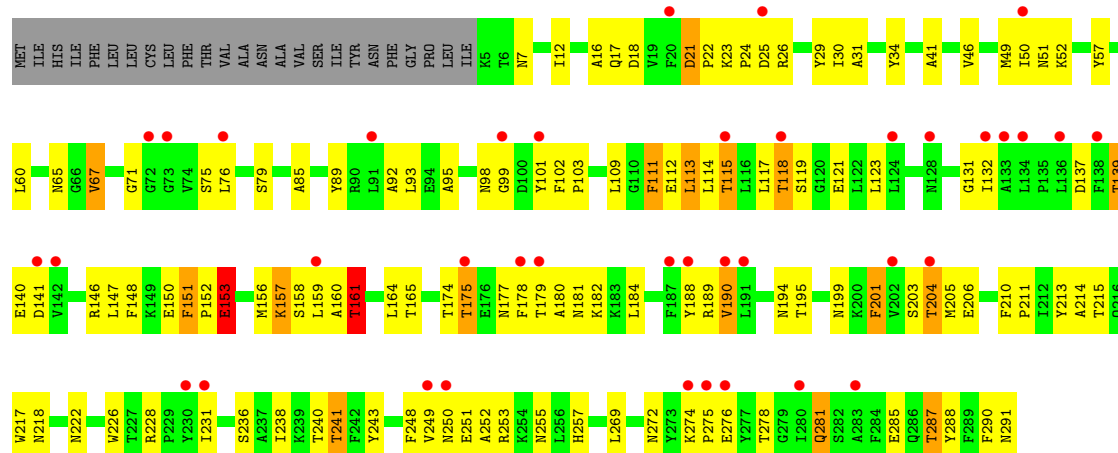




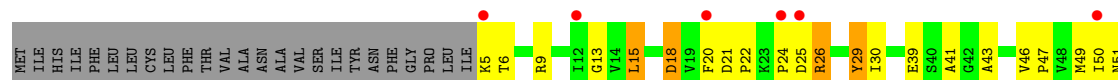
• Molecule 1: Gamma-glutamyl hydrolase

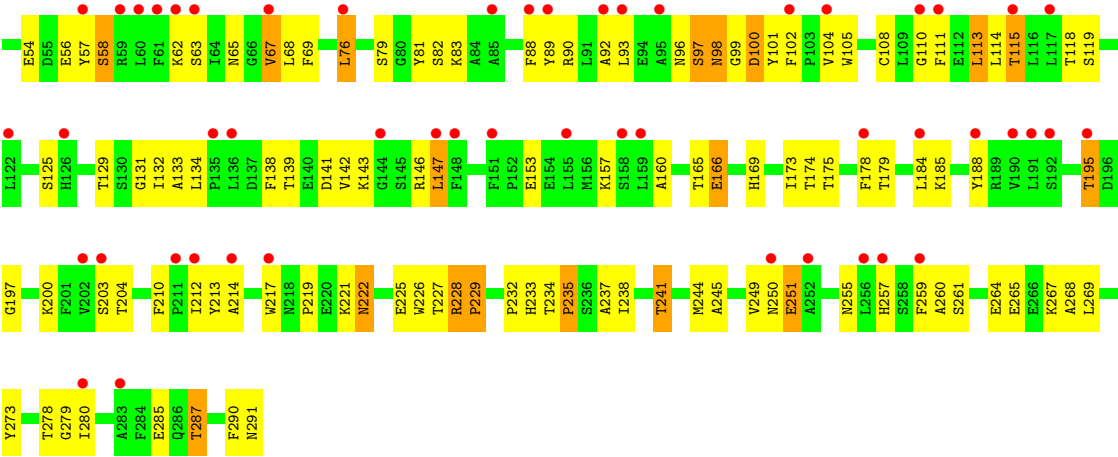


• Molecule 1: Gamma-glutamyl hydrolase



• Molecule 1: Gamma-glutamyl hydrolase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	226.50Å 61.34Å 156.96Å 90.00° 101.37° 90.00°	Depositor
Resolution (Å)	29.76 – 2.34 29.76 – 2.34	Depositor EDS
% Data completeness (in resolution range)	98.2 (29.76-2.34) 98.1 (29.76-2.34)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.87 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.239 , 0.304 (Not available) , 0.301	Depositor DCC
R_{free} test set	4494 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	43.5	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 28.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14068	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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

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

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	C	1.23	6/2371 (0.3%)	1.23	13/3217 (0.4%)
1	E	1.05	2/2371 (0.1%)	1.20	11/3217 (0.3%)
1	F	1.04	2/2371 (0.1%)	1.17	8/3217 (0.2%)
1	G	1.14	3/2371 (0.1%)	1.19	9/3217 (0.3%)
1	K	0.83	0/2371	1.05	11/3217 (0.3%)
1	M	0.85	1/2371 (0.0%)	1.08	5/3217 (0.2%)
All	All	1.03	14/14226 (0.1%)	1.15	57/19302 (0.3%)

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	E	0	2
1	M	0	1
All	All	0	3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	25	ASP	C-N	13.76	1.51	1.33
1	G	46	VAL	CA-CB	6.34	1.59	1.54
1	F	41	ALA	CA-CB	-6.03	1.43	1.53
1	G	132	ILE	CA-CB	5.98	1.61	1.55
1	E	291	ASN	C-OXT	-5.91	1.11	1.23
1	G	36	LYS	C-O	-5.80	1.17	1.24
1	C	26	ARG	C-O	-5.63	1.19	1.24
1	C	62	LYS	CA-C	-5.61	1.45	1.52
1	C	51	ASN	N-CA	5.60	1.53	1.46
1	C	228	ARG	N-CA	-5.53	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	35	VAL	CA-CB	5.32	1.60	1.54
1	C	34	TYR	N-CA	5.22	1.52	1.46
1	M	280	ILE	CA-CB	5.16	1.59	1.54
1	C	249	VAL	CA-C	5.09	1.60	1.52

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	25	ASP	CA-C-N	14.96	144.07	122.24
1	E	25	ASP	C-N-CA	14.96	144.07	122.24
1	E	25	ASP	O-C-N	-12.65	105.76	122.59
1	F	50	ILE	CA-C-N	-8.64	110.43	122.87
1	F	50	ILE	C-N-CA	-8.64	110.43	122.87
1	F	50	ILE	N-CA-C	8.25	119.99	111.00
1	K	50	ILE	N-CA-C	7.82	118.57	110.36
1	M	279	GLY	N-CA-C	7.58	123.17	113.24
1	M	229	PRO	CA-C-O	7.49	128.82	118.86
1	G	67	VAL	CB-CA-C	-7.48	99.18	110.55
1	F	21	ASP	CA-C-N	7.23	127.22	119.78
1	F	21	ASP	C-N-CA	7.23	127.22	119.78
1	M	26	ARG	N-CA-C	6.58	118.46	109.11
1	K	17	GLN	N-CA-C	6.48	119.17	108.99
1	C	50	ILE	CA-C-N	-6.47	109.19	121.54
1	C	50	ILE	C-N-CA	-6.47	109.19	121.54
1	K	132	ILE	N-CA-C	6.37	116.21	108.06
1	F	280	ILE	CB-CA-C	-6.11	103.89	112.14
1	E	196	ASP	N-CA-C	-6.02	105.52	112.92
1	C	188	TYR	N-CA-C	6.00	118.73	109.07
1	C	67	VAL	CB-CA-C	-6.00	99.97	110.71
1	K	51	ASN	N-CA-C	5.97	118.33	108.49
1	C	284	PHE	N-CA-C	5.94	118.20	108.52
1	F	45	VAL	N-CA-C	5.81	116.85	108.48
1	C	50	ILE	N-CA-C	5.64	120.31	112.35
1	K	218	ASN	CA-C-N	5.55	124.75	118.97
1	K	218	ASN	C-N-CA	5.55	124.75	118.97
1	G	50	ILE	N-CA-C	5.51	115.75	110.74
1	E	231	ILE	CA-C-N	5.47	126.31	120.13
1	E	231	ILE	C-N-CA	5.47	126.31	120.13
1	E	12	ILE	N-CA-C	5.44	115.72	108.11
1	G	259	PHE	N-CA-C	-5.42	102.49	110.52
1	G	134	LEU	CA-C-N	5.41	125.71	119.92
1	G	134	LEU	C-N-CA	5.41	125.71	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	145	SER	N-CA-C	5.40	117.65	110.53
1	M	174	THR	N-CA-C	-5.37	103.40	110.43
1	C	230	TYR	CA-C-N	-5.36	118.73	122.59
1	C	230	TYR	C-N-CA	-5.36	118.73	122.59
1	C	142	VAL	CB-CA-C	-5.35	103.59	112.26
1	K	140	GLU	N-CA-C	-5.31	106.06	112.54
1	E	44	ARG	N-CA-C	-5.31	101.46	109.85
1	G	49	MET	N-CA-C	5.28	117.35	110.43
1	C	262	THR	N-CA-C	-5.26	105.62	111.36
1	K	214	ALA	N-CA-C	5.21	117.17	108.99
1	F	201	PHE	N-CA-C	5.18	118.04	109.85
1	C	275	PRO	CA-C-N	-5.15	114.72	122.81
1	C	275	PRO	C-N-CA	-5.15	114.72	122.81
1	K	201	PHE	N-CA-C	5.15	117.63	109.50
1	E	279	GLY	N-CA-C	5.15	120.39	114.16
1	E	15	LEU	N-CA-C	5.14	117.12	109.25
1	G	142	VAL	CB-CA-C	-5.14	104.19	112.16
1	K	21	ASP	CA-C-N	5.14	125.13	119.89
1	K	21	ASP	C-N-CA	5.14	125.13	119.89
1	M	229	PRO	N-CA-C	-5.12	107.06	114.18
1	G	9	ARG	CA-C-N	5.10	125.01	119.76
1	G	9	ARG	C-N-CA	5.10	125.01	119.76
1	C	228	ARG	N-CA-C	-5.02	100.36	109.09

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	144	GLY	Peptide
1	E	25	ASP	Mainchain
1	M	228	ARG	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2307	0	2228	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2307	0	2228	53	0
1	F	2307	0	2228	68	0
1	G	2307	0	2228	84	0
1	K	2307	0	2228	93	0
1	M	2307	0	2228	113	0
2	C	6	0	8	0	0
2	G	6	0	8	0	0
2	K	6	0	8	0	0
3	C	63	0	0	2	0
3	E	43	0	0	0	0
3	F	39	0	0	1	0
3	G	40	0	0	2	0
3	K	11	0	0	6	0
3	M	12	0	0	1	0
All	All	14068	0	13392	455	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 17.

All (455) 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:K:123:LEU:HG	3:K:407:HOH:O	1.35	1.22
1:G:51:ASN:HA	3:G:423:HOH:O	1.45	1.15
1:G:89:TYR:OH	1:G:118:THR:HG22	1.54	1.08
1:E:140:GLU:HA	1:E:140:GLU:OE2	1.60	1.02
1:K:137:ASP:HA	3:K:404:HOH:O	1.62	0.99
1:G:195:THR:HG23	1:M:197:GLY:HA2	1.44	0.99
1:M:118:THR:HG21	1:M:188:TYR:HE2	1.25	0.98
1:F:25:ASP:H	1:F:291:ASN:HD22	1.14	0.92
1:F:255:ASN:ND2	1:F:257:HIS:H	1.69	0.89
1:C:139:THR:O	1:C:142:VAL:HG23	1.71	0.88
1:F:222:ASN:HB2	1:F:241:THR:HG21	1.54	0.87
1:F:222:ASN:HB2	1:F:241:THR:CG2	2.05	0.86
1:E:118:THR:HG21	1:E:188:TYR:OH	1.75	0.86
1:M:118:THR:HG21	1:M:188:TYR:CE2	2.13	0.84
1:E:24:PRO:O	1:E:25:ASP:HB2	1.76	0.84
1:C:222:ASN:HB2	1:C:241:THR:CG2	2.08	0.83
1:C:56:GLU:OE2	1:C:59:ARG:HD3	1.79	0.82
1:K:111:PHE:C	1:K:111:PHE:CD2	2.57	0.81
1:G:65:ASN:HD22	1:G:255:ASN:HD22	1.27	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:49:MET:HE3	1:F:49:MET:HA	1.61	0.81
1:M:138:PHE:HE1	1:M:160:ALA:HB2	1.46	0.80
1:C:20:PHE:O	1:C:22:PRO:HD3	1.82	0.80
1:E:50:ILE:HD11	1:E:81:TYR:HA	1.64	0.78
1:K:24:PRO:O	1:K:25:ASP:HB2	1.82	0.77
1:M:115:THR:HA	1:M:184:LEU:HD21	1.66	0.77
1:E:89:TYR:OH	1:E:118:THR:HG22	1.85	0.76
1:C:139:THR:O	1:C:142:VAL:CG2	2.32	0.76
1:M:65:ASN:HD22	1:M:255:ASN:HD22	1.34	0.76
1:M:24:PRO:O	1:M:25:ASP:HB2	1.86	0.75
1:G:7:ASN:O	1:G:253:ARG:HG2	1.85	0.75
1:F:118:THR:HG21	1:F:188:TYR:OH	1.86	0.75
1:M:15:LEU:HD12	1:M:69:PHE:CD2	2.22	0.74
1:M:89:TYR:O	1:M:93:LEU:HG	1.86	0.74
1:C:16:ALA:O	1:C:50:ILE:HD13	1.88	0.74
1:E:118:THR:CG2	1:E:188:TYR:OH	2.35	0.74
1:F:199:ASN:HA	3:F:404:HOH:O	1.86	0.73
1:K:165:THR:HB	1:K:217:TRP:CE3	2.23	0.73
1:K:121:GLU:C	3:K:407:HOH:O	2.31	0.73
1:F:255:ASN:HD21	1:F:257:HIS:CG	2.07	0.72
1:C:118:THR:HG21	1:C:188:TYR:OH	1.90	0.71
1:M:54:GLU:CD	1:M:90:ARG:HH22	1.98	0.71
1:K:255:ASN:OD1	1:K:257:HIS:CD2	2.43	0.71
1:K:111:PHE:HD2	1:K:112:GLU:N	1.87	0.71
1:M:138:PHE:CE1	1:M:160:ALA:HB2	2.26	0.70
1:G:58:SER:O	1:G:62:LYS:HG3	1.89	0.70
1:K:189:ARG:O	1:K:205:MET:HB2	1.91	0.70
1:M:119:SER:HB3	1:M:184:LEU:HG	1.73	0.70
1:E:263:GLU:O	1:E:267:LYS:HD3	1.90	0.70
1:K:111:PHE:C	1:K:111:PHE:HD2	1.99	0.70
1:M:165:THR:HG22	1:M:217:TRP:CE3	2.28	0.69
1:M:259:PHE:HD2	1:M:264:GLU:HG3	1.58	0.69
1:F:68:LEU:C	1:F:68:LEU:HD23	2.18	0.69
1:M:41:ALA:HB2	1:M:245:ALA:HB1	1.73	0.69
1:M:30:ILE:HG13	1:M:290:PHE:HE1	1.57	0.69
1:M:67:VAL:HG23	1:M:104:VAL:HG22	1.75	0.68
1:G:124:LEU:HD23	1:G:173:ILE:HD11	1.75	0.68
1:F:18:ASP:CG	1:F:50:ILE:HD11	2.19	0.68
1:M:13:GLY:HA2	1:M:46:VAL:O	1.94	0.68
1:G:124:LEU:HD23	1:G:173:ILE:CD1	2.24	0.67
1:K:46:VAL:HG11	1:K:60:LEU:HD11	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:222:ASN:HB2	1:C:241:THR:HG21	1.73	0.67
1:C:56:GLU:OE2	1:C:59:ARG:CD	2.42	0.67
1:M:166:GLU:HG2	1:M:221:LYS:HD2	1.75	0.67
1:G:259:PHE:CD1	1:G:265:GLU:HG3	2.29	0.67
1:E:42:GLY:HA3	1:F:238:ILE:HD13	1.76	0.66
1:M:219:PRO:O	1:M:241:THR:HB	1.95	0.66
1:M:255:ASN:HD21	1:M:257:HIS:HB2	1.60	0.66
1:K:85:ALA:HB3	1:K:113:LEU:HD11	1.78	0.66
1:K:23:LYS:O	1:K:26:ARG:N	2.29	0.65
1:K:25:ASP:O	1:K:26:ARG:HG2	1.96	0.65
1:M:100:ASP:OD1	1:M:101:TYR:N	2.29	0.65
1:G:65:ASN:HD22	1:G:255:ASN:ND2	1.94	0.65
1:G:56:GLU:HG3	1:G:59:ARG:NH2	2.12	0.65
1:K:204:THR:HG23	1:K:215:THR:HG22	1.78	0.65
1:E:253:ARG:NH2	1:F:238:ILE:CD1	2.59	0.65
1:C:138:PHE:HB3	1:C:142:VAL:HG21	1.79	0.65
1:G:195:THR:CG2	1:M:197:GLY:HA2	2.25	0.65
1:G:204:THR:HG23	1:G:215:THR:HG22	1.78	0.64
1:F:227:THR:HG21	1:F:282:SER:O	1.97	0.64
1:F:68:LEU:HD23	1:F:69:PHE:N	2.13	0.63
1:G:136:LEU:HD22	1:G:192:SER:OG	1.98	0.63
1:F:15:LEU:N	1:F:15:LEU:HD23	2.13	0.63
1:E:46:VAL:HG13	1:E:268:ALA:O	1.99	0.63
1:G:62:LYS:O	1:G:257:HIS:HB3	1.98	0.63
1:F:24:PRO:C	1:F:26:ARG:H	2.07	0.62
1:M:67:VAL:HG22	1:M:102:PHE:CE2	2.33	0.62
1:E:188:TYR:CE1	1:E:205:MET:HE3	2.34	0.62
1:G:56:GLU:HA	1:G:59:ARG:CZ	2.29	0.62
1:K:278:THR:OG1	1:K:287:THR:HG23	1.99	0.62
1:M:67:VAL:HG22	1:M:102:PHE:HE2	1.65	0.62
1:K:29:TYR:HA	1:K:288:TYR:O	1.99	0.62
1:M:227:THR:O	1:M:228:ARG:HD3	1.98	0.62
1:G:39:GLU:HA	1:G:43:ALA:O	1.99	0.62
1:E:44:ARG:HD3	1:F:226:TRP:CD1	2.35	0.61
1:E:140:GLU:OE2	1:E:140:GLU:CA	2.39	0.61
1:F:65:ASN:HD22	1:F:255:ASN:HD22	1.47	0.61
1:M:65:ASN:ND2	1:M:255:ASN:HD22	1.97	0.61
1:G:138:PHE:CD2	1:G:142:VAL:HG11	2.36	0.61
1:M:41:ALA:HB3	1:M:249:VAL:HG21	1.83	0.61
1:E:278:THR:HA	1:E:281:GLN:HE22	1.66	0.60
1:K:71:GLY:HA2	1:K:109:LEU:HB3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:250:ASN:ND2	1:C:253:ARG:HH11	1.99	0.60
1:M:227:THR:O	1:M:228:ARG:NH1	2.30	0.60
1:M:57:TYR:HD2	1:M:88:PHE:HE1	1.47	0.60
1:M:249:VAL:C	1:M:251:GLU:H	2.10	0.60
1:G:89:TYR:HH	1:G:118:THR:HG22	1.64	0.59
1:M:81:TYR:CE2	1:M:113:LEU:CD1	2.86	0.59
1:M:278:THR:OG1	1:M:287:THR:HG23	2.01	0.59
1:K:178:PHE:C	1:K:180:ALA:H	2.09	0.59
1:F:222:ASN:HB2	1:F:241:THR:HG22	1.85	0.59
1:G:16:ALA:HA	1:G:30:ILE:HG13	1.85	0.59
1:M:81:TYR:CE2	1:M:113:LEU:HD12	2.37	0.58
1:C:16:ALA:O	1:C:50:ILE:CD1	2.51	0.58
1:K:217:TRP:CD1	1:K:217:TRP:H	2.18	0.58
1:K:157:LYS:O	1:K:159:LEU:N	2.36	0.58
1:C:165:THR:HB	1:C:217:TRP:CE3	2.37	0.58
1:G:26:ARG:HH21	1:G:276:GLU:CD	2.11	0.58
1:C:50:ILE:HD11	1:C:81:TYR:HA	1.84	0.58
1:M:62:LYS:O	1:M:257:HIS:HB3	2.03	0.58
1:E:114:LEU:O	1:E:118:THR:HG23	2.04	0.58
1:M:222:ASN:HB3	1:M:232:PRO:O	2.04	0.58
1:M:96:ASN:C	1:M:98:ASN:H	2.11	0.57
1:G:56:GLU:CG	1:G:59:ARG:HH22	2.16	0.57
1:M:147:LEU:HD12	1:M:213:TYR:HD2	1.69	0.57
1:K:160:ALA:O	1:K:161:THR:HG23	2.04	0.57
1:M:92:ALA:O	1:M:96:ASN:HB2	2.05	0.57
1:F:255:ASN:HD21	1:F:257:HIS:H	1.51	0.57
1:G:173:ILE:O	1:G:201:PHE:HB2	2.03	0.57
1:K:189:ARG:HG2	1:K:190:VAL:N	2.20	0.57
1:E:50:ILE:O	1:E:57:TYR:OH	2.21	0.57
1:C:26:ARG:NH2	1:C:276:GLU:OE1	2.34	0.57
1:E:217:TRP:H	1:E:217:TRP:CD1	2.22	0.57
1:C:285:GLU:HG3	1:G:271:TYR:CE1	2.39	0.57
1:F:49:MET:HE3	1:F:49:MET:CA	2.34	0.56
1:F:217:TRP:CD1	1:F:217:TRP:H	2.21	0.56
1:K:189:ARG:HG2	1:K:190:VAL:H	1.70	0.56
1:M:195:THR:HG23	1:M:197:GLY:H	1.70	0.56
1:M:217:TRP:H	1:M:217:TRP:CD1	2.23	0.56
1:F:100:ASP:OD2	1:F:257:HIS:NE2	2.35	0.56
1:C:140:GLU:HG3	3:C:415:HOH:O	2.05	0.56
1:F:87:ILE:HD13	1:F:90:ARG:HH12	1.71	0.56
1:G:222:ASN:HB2	1:G:241:THR:HG22	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:118:THR:HG21	1:K:188:TYR:OH	2.06	0.56
1:K:178:PHE:C	1:K:180:ALA:N	2.62	0.56
1:M:81:TYR:HE2	1:M:113:LEU:HD12	1.71	0.56
1:M:261:SER:O	1:M:264:GLU:HG2	2.06	0.56
1:F:37:PHE:CE2	1:F:245:ALA:HB2	2.42	0.55
1:G:278:THR:OG1	1:G:287:THR:HG23	2.06	0.55
1:G:56:GLU:CG	1:G:59:ARG:NH2	2.70	0.55
1:K:103:PRO:HA	1:K:211:PRO:HB2	1.88	0.55
1:C:17:GLN:OE1	1:C:72:GLY:HA3	2.07	0.55
1:K:151:PHE:HB2	1:K:156:MET:HG2	1.88	0.54
1:M:30:ILE:HG13	1:M:290:PHE:CE1	2.41	0.54
1:G:87:ILE:HD13	1:G:90:ARG:HH22	1.73	0.54
1:K:67:VAL:HG22	1:K:102:PHE:HE2	1.72	0.54
1:M:104:VAL:HB	1:M:212:ILE:HG12	1.89	0.54
1:F:231:ILE:HG22	1:F:233:HIS:CE1	2.43	0.54
1:K:49:MET:HE2	1:K:49:MET:HA	1.90	0.54
1:K:226:TRP:HB2	1:K:285:GLU:OE1	2.08	0.54
1:M:41:ALA:CB	1:M:249:VAL:HG21	2.38	0.54
1:F:219:PRO:O	1:F:241:THR:HB	2.07	0.54
1:E:278:THR:OG1	1:E:287:THR:CG2	2.57	0.53
1:G:222:ASN:HB2	1:G:241:THR:CG2	2.38	0.53
1:M:111:PHE:HD1	1:M:214:ALA:HB1	1.74	0.53
1:C:114:LEU:O	1:C:118:THR:HG23	2.08	0.53
1:M:138:PHE:HE1	1:M:160:ALA:CB	2.20	0.53
1:M:111:PHE:CD1	1:M:214:ALA:HB1	2.44	0.53
1:M:115:THR:CA	1:M:184:LEU:HD21	2.36	0.53
1:F:89:TYR:OH	1:F:118:THR:HG22	2.08	0.53
1:K:85:ALA:CB	1:K:113:LEU:CD1	2.87	0.53
1:E:118:THR:HG21	1:E:188:TYR:CZ	2.43	0.53
1:G:55:ASP:O	1:G:59:ARG:HG3	2.08	0.53
1:G:118:THR:HG21	1:G:188:TYR:OH	2.09	0.53
1:K:148:PHE:HA	1:K:151:PHE:CE1	2.44	0.53
1:K:159:LEU:HA	1:K:164:LEU:HD12	1.91	0.53
1:M:114:LEU:O	1:M:118:THR:HG22	2.09	0.53
1:F:49:MET:HA	1:F:49:MET:CE	2.33	0.52
1:C:24:PRO:O	1:C:25:ASP:HB2	2.09	0.52
1:C:59:ARG:HH11	1:C:59:ARG:CG	2.22	0.52
1:G:17:GLN:OE1	1:G:72:GLY:HA3	2.09	0.52
1:C:111:PHE:C	1:C:111:PHE:CD2	2.88	0.52
1:F:25:ASP:H	1:F:291:ASN:ND2	1.94	0.52
1:G:213:TYR:OH	1:G:251:GLU:OE2	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:253:ARG:NH2	1:F:238:ILE:HD12	2.25	0.52
1:F:24:PRO:C	1:F:26:ARG:N	2.68	0.52
1:F:173:ILE:HG12	1:F:173:ILE:O	2.09	0.52
1:C:219:PRO:O	1:C:241:THR:HB	2.10	0.52
1:M:249:VAL:O	1:M:251:GLU:N	2.43	0.52
1:C:32:ALA:O	1:C:36:LYS:HG3	2.09	0.52
1:K:121:GLU:HB2	3:K:407:HOH:O	2.09	0.52
1:K:236:SER:O	1:K:240:THR:OG1	2.27	0.52
1:M:134:LEU:O	1:M:165:THR:OG1	2.20	0.52
1:G:173:ILE:HG22	1:G:174:THR:O	2.10	0.51
1:G:255:ASN:HD21	1:G:257:HIS:CG	2.28	0.51
1:M:98:ASN:O	1:M:100:ASP:N	2.43	0.51
1:M:146:ARG:NH2	1:M:210:PHE:O	2.42	0.51
1:F:278:THR:OG1	1:F:287:THR:CG2	2.58	0.51
1:C:218:ASN:ND2	3:C:419:HOH:O	2.43	0.51
1:G:56:GLU:HG2	1:G:59:ARG:HH22	1.76	0.51
1:F:278:THR:HG21	1:F:287:THR:HG23	1.93	0.51
1:F:115:THR:HG21	1:F:173:ILE:HD12	1.91	0.51
1:M:222:ASN:HD22	1:M:241:THR:HG22	1.76	0.51
1:G:217:TRP:H	1:G:217:TRP:CD1	2.28	0.51
1:C:39:GLU:HA	1:C:43:ALA:O	2.10	0.51
1:M:165:THR:HG22	1:M:217:TRP:CZ3	2.44	0.51
1:C:217:TRP:H	1:C:217:TRP:CD1	2.28	0.51
1:E:221:LYS:HG2	1:E:225:GLU:HG3	1.93	0.51
1:M:65:ASN:HA	1:M:255:ASN:ND2	2.26	0.51
1:E:100:ASP:OD1	1:E:100:ASP:C	2.52	0.50
1:G:36:LYS:HZ1	1:G:286:GLN:NE2	2.09	0.50
1:G:111:PHE:C	1:G:111:PHE:CD2	2.89	0.50
1:C:20:PHE:C	1:C:22:PRO:HD3	2.36	0.50
1:G:255:ASN:ND2	1:G:257:HIS:H	2.09	0.50
1:M:90:ARG:HA	1:M:93:LEU:HD12	1.94	0.50
1:E:37:PHE:CE2	1:E:245:ALA:HB2	2.46	0.50
1:G:170:GLN:HB3	1:G:171:TRP:CD1	2.45	0.50
1:K:119:SER:HB3	1:K:184:LEU:HD21	1.93	0.50
1:F:112:GLU:O	1:F:115:THR:OG1	2.28	0.50
1:G:278:THR:OG1	1:G:287:THR:CG2	2.60	0.50
1:K:248:PHE:O	1:K:251:GLU:HB2	2.12	0.50
1:C:278:THR:OG1	1:C:287:THR:HG23	2.12	0.50
1:M:111:PHE:C	1:M:111:PHE:CD2	2.90	0.49
1:M:108:CYS:O	1:M:111:PHE:HB3	2.12	0.49
1:F:114:LEU:O	1:F:118:THR:HG23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:250:ASN:ND2	1:K:253:ARG:HH11	2.09	0.49
1:E:16:ALA:HB1	1:E:28:SER:HB2	1.93	0.49
1:F:139:THR:HG21	1:F:190:VAL:HG12	1.93	0.49
1:M:115:THR:HA	1:M:184:LEU:CD2	2.38	0.49
1:K:255:ASN:HD21	1:K:257:HIS:CD2	2.31	0.49
1:K:85:ALA:HB3	1:K:113:LEU:CD1	2.41	0.49
1:K:93:LEU:HA	1:K:210:PHE:CE1	2.47	0.49
1:K:243:TYR:HD2	3:K:401:HOH:O	1.96	0.49
1:G:53:SER:N	1:G:56:GLU:OE1	2.34	0.49
1:C:118:THR:CG2	1:C:188:TYR:OH	2.60	0.49
1:E:67:VAL:HG22	1:E:102:PHE:HE2	1.77	0.48
1:K:178:PHE:O	1:K:180:ALA:N	2.46	0.48
1:G:166:GLU:CD	1:G:221:LYS:HD2	2.38	0.48
1:G:26:ARG:NH2	1:G:276:GLU:OE1	2.47	0.48
1:K:228:ARG:HB2	1:K:231:ILE:HD11	1.95	0.48
1:K:121:GLU:HB2	3:K:408:HOH:O	2.11	0.48
1:K:152:PRO:O	1:K:153:GLU:C	2.56	0.48
1:M:234:THR:H	1:M:237:ALA:HB3	1.78	0.48
1:G:178:PHE:CE1	1:G:184:LEU:HB3	2.49	0.48
1:K:31:ALA:HB3	1:K:34:TYR:CD1	2.48	0.48
1:C:225:GLU:OE2	1:C:225:GLU:HA	2.14	0.48
1:C:248:PHE:O	1:C:251:GLU:HB2	2.13	0.48
1:G:89:TYR:CZ	1:G:118:THR:HG22	2.45	0.48
1:K:93:LEU:HA	1:K:210:PHE:HE1	1.79	0.48
1:K:139:THR:HB	1:K:141:ASP:H	1.78	0.48
1:F:255:ASN:HD21	1:F:257:HIS:CB	2.26	0.47
1:C:228:ARG:HG3	1:C:230:TYR:OH	2.13	0.47
1:G:126:HIS:HE1	1:G:170:GLN:HG2	1.79	0.47
1:M:79:SER:O	1:M:82:SER:OG	2.31	0.47
1:F:111:PHE:CE1	1:F:205:MET:HE2	2.48	0.47
1:G:278:THR:HG21	1:G:287:THR:HG23	1.96	0.47
1:E:44:ARG:HD3	1:F:226:TRP:CG	2.48	0.47
1:G:139:THR:O	1:G:142:VAL:HG22	2.14	0.47
1:K:181:ASN:HD22	1:K:182:LYS:N	2.12	0.47
1:K:195:THR:HA	1:K:199:ASN:O	2.14	0.47
1:F:118:THR:HG21	1:F:188:TYR:CZ	2.48	0.47
1:C:16:ALA:HA	1:C:30:ILE:HG13	1.96	0.47
1:C:89:TYR:OH	1:C:118:THR:HB	2.13	0.47
1:M:50:ILE:HG23	1:M:51:ASN:N	2.29	0.47
1:K:16:ALA:HA	1:K:30:ILE:CG1	2.45	0.47
1:M:57:TYR:CD2	1:M:88:PHE:HE1	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:111:PHE:HE1	1:F:205:MET:HG2	1.79	0.47
1:E:141:ASP:OD1	1:E:141:ASP:N	2.44	0.47
1:F:105:TRP:CE3	1:F:213:TYR:HB2	2.50	0.47
1:F:280:ILE:HB	1:F:281:GLN:HG2	1.97	0.47
1:G:36:LYS:NZ	1:G:286:GLN:NE2	2.63	0.47
1:M:49:MET:HE1	1:M:291:ASN:OXT	2.14	0.47
1:E:225:GLU:O	1:E:233:HIS:HE1	1.98	0.47
1:E:278:THR:HG21	1:E:287:THR:HG23	1.97	0.47
1:C:188:TYR:CE1	1:C:205:MET:HE3	2.50	0.47
1:M:129:THR:OG1	1:M:169:HIS:O	2.23	0.47
1:E:253:ARG:HH22	1:F:238:ILE:HD13	1.80	0.46
1:C:250:ASN:ND2	1:C:253:ARG:NH1	2.62	0.46
1:K:65:ASN:HB3	1:K:255:ASN:HB3	1.97	0.46
1:M:259:PHE:CD2	1:M:264:GLU:HG3	2.44	0.46
1:F:111:PHE:C	1:F:111:PHE:CD2	2.93	0.46
1:G:219:PRO:O	1:G:241:THR:HB	2.15	0.46
1:M:105:TRP:HH2	1:M:244:MET:HE3	1.80	0.46
1:M:166:GLU:CG	1:M:221:LYS:HD2	2.42	0.46
1:M:178:PHE:CE1	1:M:184:LEU:HB3	2.50	0.46
1:G:186:LYS:O	1:G:186:LYS:HD3	2.16	0.46
1:M:76:LEU:HD23	1:M:76:LEU:N	2.31	0.46
1:E:253:ARG:NH2	1:F:238:ILE:HD13	2.31	0.46
1:C:285:GLU:OE2	1:C:285:GLU:HA	2.13	0.46
1:G:60:LEU:HD23	1:G:60:LEU:O	2.16	0.46
1:K:111:PHE:CD2	1:K:112:GLU:N	2.73	0.46
1:K:146:ARG:NH2	1:K:213:TYR:OH	2.49	0.46
1:M:21:ASP:O	1:M:22:PRO:C	2.59	0.46
1:G:186:LYS:HD3	1:G:186:LYS:C	2.41	0.46
1:M:178:PHE:O	1:M:179:THR:C	2.58	0.46
1:G:166:GLU:CG	1:G:221:LYS:HD2	2.45	0.46
1:K:228:ARG:HB2	1:K:231:ILE:CD1	2.46	0.46
1:M:118:THR:HG23	1:M:184:LEU:HD23	1.97	0.46
1:F:30:ILE:HG22	1:F:31:ALA:O	2.16	0.46
1:C:285:GLU:HG3	1:G:271:TYR:CZ	2.51	0.46
1:M:68:LEU:HA	1:M:105:TRP:O	2.16	0.46
1:C:52:LYS:HD3	1:C:52:LYS:HA	1.68	0.46
1:G:61:PHE:C	1:G:61:PHE:CD2	2.94	0.45
1:G:266:GLU:O	1:G:272:ASN:OD1	2.34	0.45
1:K:147:LEU:HD22	1:K:148:PHE:CE1	2.51	0.45
1:K:174:THR:OG1	1:K:177:ASN:ND2	2.47	0.45
1:K:269:LEU:O	1:K:272:ASN:ND2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:15:LEU:HD12	1:M:69:PHE:CE2	2.51	0.45
1:G:16:ALA:HA	1:G:30:ILE:CG1	2.47	0.45
1:K:101:TYR:OH	1:K:251:GLU:OE2	2.31	0.45
1:C:124:LEU:HD13	1:C:171:TRP:HB3	1.98	0.45
1:M:63:SER:HB3	1:M:259:PHE:CD1	2.51	0.45
1:E:36:LYS:HB3	1:E:224:PHE:CE1	2.52	0.45
1:G:60:LEU:HD23	1:G:60:LEU:C	2.41	0.45
1:F:278:THR:CG2	1:F:287:THR:HG23	2.47	0.45
1:K:222:ASN:HB2	1:K:241:THR:CG2	2.47	0.45
1:M:56:GLU:C	1:M:58:SER:H	2.24	0.45
1:M:234:THR:H	1:M:237:ALA:CB	2.30	0.45
1:M:39:GLU:HA	1:M:43:ALA:O	2.16	0.45
1:G:111:PHE:CD2	1:G:216:GLN:NE2	2.85	0.45
1:K:178:PHE:CE1	1:K:184:LEU:HB3	2.51	0.45
1:M:46:VAL:HA	1:M:47:PRO:HD2	1.76	0.45
1:M:278:THR:CG2	1:M:287:THR:HG23	2.47	0.45
1:M:255:ASN:HD21	1:M:257:HIS:CB	2.28	0.44
1:C:25:ASP:O	1:C:26:ARG:HG2	2.16	0.44
1:G:36:LYS:NZ	1:G:286:GLN:HE21	2.15	0.44
1:M:65:ASN:HD22	1:M:255:ASN:ND2	2.08	0.44
1:F:18:ASP:OD2	1:F:50:ILE:HD11	2.18	0.44
1:F:89:TYR:CZ	1:F:118:THR:HG22	2.53	0.44
1:G:126:HIS:HB3	3:G:402:HOH:O	2.17	0.44
1:K:114:LEU:O	1:K:115:THR:C	2.60	0.44
1:F:7:ASN:O	1:F:253:ARG:HG2	2.18	0.44
1:F:113:LEU:HD13	1:F:117:LEU:CD1	2.47	0.44
1:M:259:PHE:O	1:M:260:ALA:C	2.59	0.44
1:E:7:ASN:O	1:E:253:ARG:HG2	2.17	0.44
1:C:22:PRO:O	1:C:23:LYS:HG3	2.18	0.44
1:K:7:ASN:OD1	1:K:7:ASN:C	2.61	0.44
1:E:7:ASN:OD1	1:E:7:ASN:C	2.61	0.44
1:E:278:THR:OG1	1:E:287:THR:HG23	2.18	0.44
1:M:18:ASP:CG	1:M:50:ILE:HD11	2.43	0.44
1:M:269:LEU:HD23	1:M:269:LEU:HA	1.82	0.44
1:K:146:ARG:HG3	1:K:146:ARG:HH11	1.82	0.44
1:G:100:ASP:OD1	1:G:100:ASP:C	2.61	0.43
1:K:21:ASP:HA	1:K:22:PRO:HD2	1.86	0.43
1:K:165:THR:HB	1:K:217:TRP:CD2	2.53	0.43
1:F:68:LEU:HD23	1:F:69:PHE:C	2.43	0.43
1:C:62:LYS:O	1:C:257:HIS:HB3	2.17	0.43
1:G:111:PHE:CE2	1:G:216:GLN:NE2	2.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:151:PHE:HB2	1:K:156:MET:CG	2.48	0.43
1:E:217:TRP:CD1	1:E:217:TRP:N	2.87	0.43
1:M:29:TYR:CD2	1:M:29:TYR:C	2.97	0.43
1:K:75:SER:O	1:K:79:SER:OG	2.23	0.43
1:F:138:PHE:HB3	1:F:142:VAL:HG11	1.99	0.43
1:K:101:TYR:CE2	1:K:251:GLU:OE2	2.72	0.43
1:M:101:TYR:O	1:M:255:ASN:HB2	2.18	0.43
1:G:263:GLU:H	1:G:263:GLU:HG2	1.67	0.43
1:M:217:TRP:CZ3	1:M:219:PRO:HB3	2.54	0.43
1:C:105:TRP:CE3	1:C:213:TYR:HB2	2.54	0.43
1:C:118:THR:HG21	1:C:188:TYR:CZ	2.52	0.43
1:C:227:THR:O	1:C:228:ARG:HD3	2.18	0.43
1:C:228:ARG:HA	1:C:229:PRO:HD3	1.75	0.43
1:G:65:ASN:ND2	1:G:255:ASN:HD22	2.05	0.43
1:E:81:TYR:CE2	1:E:113:LEU:HD12	2.54	0.43
1:E:219:PRO:O	1:E:241:THR:HB	2.18	0.43
1:G:68:LEU:C	1:G:68:LEU:HD23	2.43	0.43
1:G:207:ALA:HB3	1:G:210:PHE:O	2.19	0.43
1:M:63:SER:HB3	1:M:259:PHE:CE1	2.53	0.43
1:M:114:LEU:O	1:M:115:THR:C	2.61	0.43
1:M:265:GLU:C	1:M:267:LYS:H	2.26	0.43
1:K:238:ILE:O	1:K:241:THR:HG23	2.19	0.43
1:M:139:THR:O	1:M:142:VAL:HG22	2.18	0.43
1:C:25:ASP:C	1:C:26:ARG:HG2	2.44	0.43
1:C:37:PHE:CE2	1:C:245:ALA:HB2	2.53	0.43
1:C:222:ASN:HB2	1:C:241:THR:HG22	1.97	0.43
1:M:90:ARG:HE	1:M:90:ARG:HB3	1.68	0.43
1:M:97:SER:N	3:M:412:HOH:O	2.51	0.43
1:G:38:LEU:HD23	1:G:38:LEU:HA	1.77	0.42
1:K:89:TYR:OH	1:K:118:THR:CG2	2.66	0.42
1:K:89:TYR:OH	1:K:118:THR:HG22	2.20	0.42
1:K:194:ASN:HB2	1:K:201:PHE:CZ	2.54	0.42
1:M:142:VAL:HG23	1:M:143:LYS:HD2	2.01	0.42
1:M:234:THR:O	1:M:235:PRO:C	2.62	0.42
1:M:278:THR:HG21	1:M:287:THR:HG23	2.01	0.42
1:E:224:PHE:CE1	1:F:40:SER:HA	2.54	0.42
1:G:105:TRP:CH2	1:G:244:MET:HE3	2.54	0.42
1:M:132:ILE:CG1	1:M:133:ALA:N	2.81	0.42
1:M:226:TRP:HB2	1:M:285:GLU:OE1	2.19	0.42
1:F:105:TRP:CD1	1:F:107:THR:HG1	2.37	0.42
1:E:89:TYR:CZ	1:E:118:THR:HG22	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:178:PHE:C	1:E:178:PHE:CD2	2.98	0.42
1:G:147:LEU:HD23	1:G:247:PHE:CD2	2.54	0.42
1:E:89:TYR:OH	1:E:118:THR:CG2	2.64	0.42
1:E:185:LYS:O	1:E:185:LYS:HG3	2.20	0.42
1:F:71:GLY:HA2	1:F:109:LEU:H	1.85	0.42
1:K:250:ASN:O	1:K:253:ARG:HB2	2.19	0.42
1:F:142:VAL:CG1	1:F:191:LEU:O	2.67	0.42
1:K:23:LYS:O	1:K:26:ARG:HB2	2.19	0.42
1:K:24:PRO:O	1:K:25:ASP:CB	2.57	0.42
1:K:146:ARG:HB2	1:K:206:GLU:OE1	2.20	0.42
1:M:81:TYR:CE2	1:M:113:LEU:HD11	2.54	0.42
1:F:16:ALA:HA	1:F:30:ILE:HG13	2.01	0.42
1:G:134:LEU:O	1:G:165:THR:OG1	2.25	0.42
1:G:166:GLU:HG2	1:G:221:LYS:HD2	2.01	0.42
1:M:46:VAL:HG22	1:M:268:ALA:O	2.20	0.42
1:E:16:ALA:O	1:E:50:ILE:HD13	2.20	0.41
1:G:56:GLU:HA	1:G:59:ARG:NH2	2.34	0.41
1:G:136:LEU:HG	1:G:165:THR:HG21	2.02	0.41
1:K:41:ALA:HB3	1:K:249:VAL:HG21	2.01	0.41
1:K:285:GLU:OE2	1:K:285:GLU:HA	2.20	0.41
1:F:49:MET:HE1	1:F:290:PHE:HB2	2.01	0.41
1:G:49:MET:HE3	1:G:50:ILE:H	1.86	0.41
1:C:228:ARG:HB3	1:C:230:TYR:CE2	2.55	0.41
1:C:279:GLY:O	1:C:280:ILE:C	2.63	0.41
1:K:52:LYS:HB2	1:K:57:TYR:CZ	2.55	0.41
1:M:228:ARG:HA	1:M:229:PRO:HD3	1.38	0.41
1:F:118:THR:CG2	1:F:188:TYR:OH	2.60	0.41
1:E:207:ALA:HB3	1:E:210:PHE:O	2.20	0.41
1:E:277:TYR:HD1	1:E:279:GLY:H	1.69	0.41
1:C:56:GLU:OE2	1:C:56:GLU:HA	2.20	0.41
1:M:225:GLU:O	1:M:233:HIS:HE1	2.03	0.41
1:E:41:ALA:HB1	1:E:246:ASN:HA	2.02	0.41
1:F:25:ASP:OD1	1:F:291:ASN:HB2	2.21	0.41
1:F:263:GLU:H	1:F:263:GLU:HG2	1.59	0.41
1:K:174:THR:O	1:K:175:THR:C	2.63	0.41
1:K:274:LYS:HA	1:K:275:PRO:HD3	1.90	0.41
1:E:108:CYS:O	1:E:111:PHE:HB3	2.21	0.41
1:E:113:LEU:HD22	1:E:117:LEU:HG	2.03	0.41
1:C:100:ASP:OD1	1:C:100:ASP:C	2.63	0.41
1:K:49:MET:HE1	1:K:290:PHE:CG	2.56	0.41
1:K:92:ALA:O	1:K:95:ALA:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:278:THR:CG2	1:E:287:THR:HG23	2.50	0.41
1:G:196:ASP:OD2	1:G:199:ASN:HB2	2.21	0.41
1:K:12:ILE:HD11	1:K:252:ALA:HB2	2.02	0.41
1:K:113:LEU:HD22	1:K:117:LEU:HG	2.02	0.41
1:M:227:THR:O	1:M:228:ARG:CD	2.68	0.41
1:M:251:GLU:OE1	1:M:251:GLU:HA	2.21	0.41
1:G:201:PHE:HD1	1:G:202:VAL:O	2.04	0.41
1:G:221:LYS:HD3	1:G:231:ILE:CD1	2.50	0.41
1:M:47:PRO:HG3	1:M:273:TYR:CE2	2.56	0.41
1:E:52:LYS:HB2	1:E:57:TYR:CZ	2.56	0.40
1:E:103:PRO:HA	1:E:211:PRO:O	2.20	0.40
1:G:122:LEU:HD23	1:G:122:LEU:HA	1.82	0.40
1:G:126:HIS:CE1	1:G:170:GLN:HG2	2.56	0.40
1:K:114:LEU:O	1:K:117:LEU:N	2.54	0.40
1:K:148:PHE:CD2	1:K:156:MET:SD	3.14	0.40
1:M:175:THR:HG21	1:M:200:LYS:HE2	2.03	0.40
1:F:178:PHE:CD2	1:F:178:PHE:C	2.99	0.40
1:C:188:TYR:CZ	1:C:205:MET:HE3	2.56	0.40
1:G:25:ASP:H	1:G:291:ASN:HD22	1.70	0.40
1:K:281:GLN:CD	1:K:281:GLN:N	2.78	0.40
1:E:98:ASN:C	1:E:100:ASP:H	2.30	0.40
1:F:282:SER:OG	1:F:283:ALA:N	2.53	0.40
1:K:213:TYR:CD1	1:K:213:TYR:N	2.89	0.40
1:M:100:ASP:OD1	1:M:100:ASP:C	2.64	0.40
1:K:181:ASN:HD22	1:K:182:LYS:H	1.69	0.40
1:M:69:PHE:O	1:M:110:GLY:HA3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	285/312 (91%)	271 (95%)	13 (5%)	1 (0%)	30	32
1	E	285/312 (91%)	264 (93%)	19 (7%)	2 (1%)	18	18
1	F	285/312 (91%)	270 (95%)	15 (5%)	0	100	100
1	G	285/312 (91%)	261 (92%)	23 (8%)	1 (0%)	30	32
1	K	285/312 (91%)	239 (84%)	36 (13%)	10 (4%)	3	1
1	M	285/312 (91%)	244 (86%)	33 (12%)	8 (3%)	4	2
All	All	1710/1872 (91%)	1549 (91%)	139 (8%)	22 (1%)	9	7

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	158	SER
1	K	161	THR
1	M	250	ASN
1	K	150	GLU
1	K	153	GLU
1	K	157	LYS
1	K	179	THR
1	M	97	SER
1	M	99	GLY
1	M	100	ASP
1	M	131	GLY
1	E	99	GLY
1	G	281	GLN
1	M	141	ASP
1	K	115	THR
1	K	175	THR
1	M	115	THR
1	M	9	ARG
1	K	99	GLY
1	C	229	PRO
1	E	131	GLY
1	K	131	GLY

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	C	250/272 (92%)	227 (91%)	23 (9%)	8	8
1	E	250/272 (92%)	227 (91%)	23 (9%)	8	8
1	F	250/272 (92%)	228 (91%)	22 (9%)	9	9
1	G	250/272 (92%)	221 (88%)	29 (12%)	5	4
1	K	250/272 (92%)	231 (92%)	19 (8%)	12	13
1	M	250/272 (92%)	221 (88%)	29 (12%)	5	4
All	All	1500/1632 (92%)	1355 (90%)	145 (10%)	8	7

All (145) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	5	LYS
1	E	50	ILE
1	E	55	ASP
1	E	67	VAL
1	E	83	LYS
1	E	97	SER
1	E	113	LEU
1	E	118	THR
1	E	122	LEU
1	E	125	SER
1	E	140	GLU
1	E	141	ASP
1	E	147	LEU
1	E	159	LEU
1	E	175	THR
1	E	179	THR
1	E	185	LYS
1	E	241	THR
1	E	264	GLU
1	E	276	GLU
1	E	280	ILE
1	E	281	GLN
1	E	287	THR
1	F	7	ASN
1	F	15	LEU
1	F	21	ASP
1	F	50	ILE
1	F	52	LYS

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Mol	Chain	Res	Type
1	F	74	VAL
1	F	113	LEU
1	F	118	THR
1	F	125	SER
1	F	141	ASP
1	F	147	LEU
1	F	166	GLU
1	F	172	SER
1	F	173	ILE
1	F	175	THR
1	F	186	LYS
1	F	227	THR
1	F	241	THR
1	F	263	GLU
1	F	281	GLN
1	F	282	SER
1	F	287	THR
1	C	5	LYS
1	C	18	ASP
1	C	50	ILE
1	C	56	GLU
1	C	58	SER
1	C	59	ARG
1	C	60	LEU
1	C	67	VAL
1	C	111	PHE
1	C	113	LEU
1	C	118	THR
1	C	142	VAL
1	C	147	LEU
1	C	154	GLU
1	C	175	THR
1	C	176	GLU
1	C	182	LYS
1	C	186	LYS
1	C	239	LYS
1	C	241	THR
1	C	281	GLN
1	C	285	GLU
1	C	287	THR
1	G	5	LYS
1	G	15	LEU

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Mol	Chain	Res	Type
1	G	17	GLN
1	G	40	SER
1	G	46	VAL
1	G	59	ARG
1	G	62	LYS
1	G	63	SER
1	G	67	VAL
1	G	74	VAL
1	G	111	PHE
1	G	113	LEU
1	G	119	SER
1	G	127	THR
1	G	140	GLU
1	G	142	VAL
1	G	143	LYS
1	G	147	LEU
1	G	150	GLU
1	G	166	GLU
1	G	182	LYS
1	G	186	LYS
1	G	204	THR
1	G	231	ILE
1	G	239	LYS
1	G	241	THR
1	G	263	GLU
1	G	267	LYS
1	G	287	THR
1	K	18	ASP
1	K	67	VAL
1	K	76	LEU
1	K	98	ASN
1	K	111	PHE
1	K	113	LEU
1	K	118	THR
1	K	139	THR
1	K	151	PHE
1	K	153	GLU
1	K	161	THR
1	K	190	VAL
1	K	203	SER
1	K	204	THR
1	K	241	THR

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Mol	Chain	Res	Type
1	K	276	GLU
1	K	281	GLN
1	K	287	THR
1	K	291	ASN
1	M	5	LYS
1	M	6	THR
1	M	15	LEU
1	M	18	ASP
1	M	20	PHE
1	M	26	ARG
1	M	29	TYR
1	M	58	SER
1	M	67	VAL
1	M	76	LEU
1	M	83	LYS
1	M	98	ASN
1	M	113	LEU
1	M	125	SER
1	M	147	LEU
1	M	153	GLU
1	M	157	LYS
1	M	166	GLU
1	M	173	ILE
1	M	185	LYS
1	M	195	THR
1	M	203	SER
1	M	204	THR
1	M	222	ASN
1	M	235	PRO
1	M	238	ILE
1	M	241	THR
1	M	251	GLU
1	M	287	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	126	HIS
1	E	199	ASN
1	E	218	ASN
1	E	250	ASN
1	E	281	GLN

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Mol	Chain	Res	Type
1	F	51	ASN
1	F	216	GLN
1	F	246	ASN
1	F	255	ASN
1	F	272	ASN
1	F	281	GLN
1	F	286	GLN
1	F	291	ASN
1	C	51	ASN
1	C	167	ASN
1	C	177	ASN
1	C	199	ASN
1	C	218	ASN
1	C	250	ASN
1	G	126	HIS
1	G	128	ASN
1	G	170	GLN
1	G	255	ASN
1	G	272	ASN
1	G	286	GLN
1	G	291	ASN
1	K	17	GLN
1	K	126	HIS
1	K	181	ASN
1	K	199	ASN
1	K	218	ASN
1	K	233	HIS
1	K	250	ASN
1	M	27	ASN
1	M	96	ASN
1	M	128	ASN
1	M	170	GLN
1	M	222	ASN
1	M	246	ASN
1	M	255	ASN
1	M	257	HIS
1	M	272	ASN
1	M	286	GLN

5.3.3 RNA ⓘ

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](#)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GOL	G	301	-	5,5,5	0.59	0	5,5,5	0.30	0
2	GOL	K	301	-	5,5,5	0.62	0	5,5,5	0.56	0
2	GOL	C	301	-	5,5,5	0.76	0	5,5,5	0.61	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	G	301	-	-	2/4/4/4	-
2	GOL	K	301	-	-	4/4/4/4	-
2	GOL	C	301	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	301	GOL	O1-C1-C2-C3
2	C	301	GOL	C1-C2-C3-O3
2	G	301	GOL	C1-C2-C3-O3
2	K	301	GOL	C1-C2-C3-O3
2	K	301	GOL	O1-C1-C2-C3
2	C	301	GOL	O1-C1-C2-O2
2	C	301	GOL	O2-C2-C3-O3
2	G	301	GOL	O2-C2-C3-O3
2	K	301	GOL	O1-C1-C2-O2
2	K	301	GOL	O2-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	C	287/312 (91%)	0.01	12 (4%)	40	46	9, 34, 51, 67	9 (3%)
1	E	287/312 (91%)	0.26	10 (3%)	47	53	19, 43, 60, 68	9 (3%)
1	F	287/312 (91%)	0.33	12 (4%)	40	46	14, 44, 62, 74	5 (1%)
1	G	287/312 (91%)	0.55	13 (4%)	38	44	15, 45, 62, 69	5 (1%)
1	K	287/312 (91%)	1.13	39 (13%)	7	7	23, 63, 80, 87	9 (3%)
1	M	287/312 (91%)	1.36	57 (19%)	3	3	27, 66, 87, 99	5 (1%)
All	All	1722/1872 (91%)	0.61	143 (8%)	17	20	9, 49, 77, 99	42 (2%)

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	250	ASN	8.3
1	F	250	ASN	7.7
1	E	179	THR	7.4
1	E	250	ASN	7.4
1	C	179	THR	7.3
1	K	179	THR	7.3
1	M	250	ASN	7.1
1	M	158	SER	6.7
1	G	250	ASN	6.7
1	F	158	SER	6.3
1	G	158	SER	6.1
1	M	280	ILE	6.0
1	M	283	ALA	5.7
1	E	283	ALA	5.7
1	G	283	ALA	5.6
1	F	283	ALA	5.5
1	K	202	VAL	5.2
1	C	250	ASN	5.0
1	K	280	ILE	4.7

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Mol	Chain	Res	Type	RSRZ
1	K	276	GLU	4.6
1	K	178	PHE	4.5
1	K	283	ALA	4.5
1	K	188	TYR	4.5
1	F	280	ILE	4.4
1	G	280	ILE	4.3
1	M	115	THR	4.0
1	M	104	VAL	3.8
1	C	50	ILE	3.7
1	C	283	ALA	3.5
1	E	128	ASN	3.4
1	C	202	VAL	3.3
1	K	136	LEU	3.2
1	E	280	ILE	3.2
1	C	128	ASN	3.2
1	K	72	GLY	3.1
1	K	191	LEU	3.1
1	M	184	LEU	3.1
1	C	280	ILE	3.1
1	M	257	HIS	3.1
1	M	178	PHE	3.1
1	K	25	ASP	3.1
1	M	24	PRO	3.1
1	F	198	TYR	3.0
1	K	274	LYS	3.0
1	M	126	HIS	3.0
1	G	188	TYR	3.0
1	K	50	ILE	2.9
1	M	195	THR	2.9
1	K	275	PRO	2.9
1	M	136	LEU	2.9
1	E	202	VAL	2.9
1	C	115	THR	2.9
1	G	115	THR	2.9
1	K	128	ASN	2.9
1	K	187	PHE	2.9
1	M	25	ASP	2.9
1	M	102	PHE	2.8
1	K	76	LEU	2.8
1	M	76	LEU	2.8
1	M	122	LEU	2.8
1	M	20	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	M	92	ALA	2.8
1	G	120	GLY	2.8
1	M	57	TYR	2.8
1	M	85	ALA	2.8
1	F	188	TYR	2.7
1	K	138	PHE	2.7
1	M	148	PHE	2.7
1	M	202	VAL	2.7
1	M	217	TRP	2.7
1	K	99	GLY	2.6
1	M	159	LEU	2.6
1	M	190	VAL	2.6
1	M	62	LYS	2.5
1	F	50	ILE	2.5
1	M	50	ILE	2.5
1	M	89	TYR	2.5
1	C	276	GLU	2.5
1	K	133	ALA	2.5
1	E	115	THR	2.5
1	M	259	PHE	2.5
1	E	277	TYR	2.5
1	G	198	TYR	2.5
1	K	142	VAL	2.4
1	F	134	LEU	2.4
1	K	230	TYR	2.4
1	C	274	LYS	2.4
1	M	59	ARG	2.4
1	K	115	THR	2.4
1	K	175	THR	2.4
1	G	20	PHE	2.4
1	G	50	ILE	2.4
1	M	12	ILE	2.4
1	M	188	TYR	2.4
1	M	95	ALA	2.4
1	F	115	THR	2.4
1	M	203	SER	2.4
1	K	118	THR	2.4
1	M	5	LYS	2.4
1	K	73	GLY	2.3
1	G	76	LEU	2.3
1	M	256	LEU	2.3
1	M	63	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	M	88	PHE	2.3
1	M	135	PRO	2.3
1	K	190	VAL	2.3
1	K	91	LEU	2.3
1	M	147	LEU	2.3
1	M	155	LEU	2.3
1	K	141	ASP	2.3
1	F	136	LEU	2.2
1	K	20	PHE	2.2
1	C	281	GLN	2.2
1	E	50	ILE	2.2
1	M	211	PRO	2.2
1	K	231	ILE	2.2
1	M	67	VAL	2.2
1	G	195	THR	2.2
1	M	214	ALA	2.2
1	C	230	TYR	2.2
1	K	124	LEU	2.2
1	E	20	PHE	2.2
1	M	111	PHE	2.2
1	K	134	LEU	2.1
1	M	212	ILE	2.1
1	K	249	VAL	2.1
1	M	144	GLY	2.1
1	K	204	THR	2.1
1	K	101	TYR	2.1
1	M	191	LEU	2.1
1	M	110	GLY	2.1
1	F	173	ILE	2.1
1	K	132	ILE	2.1
1	K	159	LEU	2.1
1	M	60	LEU	2.1
1	M	93	LEU	2.1
1	M	117	LEU	2.1
1	M	151	PHE	2.1
1	M	61	PHE	2.1
1	F	229	PRO	2.0
1	M	192	SER	2.0
1	M	252	ALA	2.0
1	G	173	ILE	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	K	301	6/6	0.70	0.15	66,67,67,68	0
2	GOL	C	301	6/6	0.75	0.19	62,69,70,70	0
2	GOL	G	301	6/6	0.84	0.17	55,59,59,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.