



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:13 am GMT

PDB ID : 4L95
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

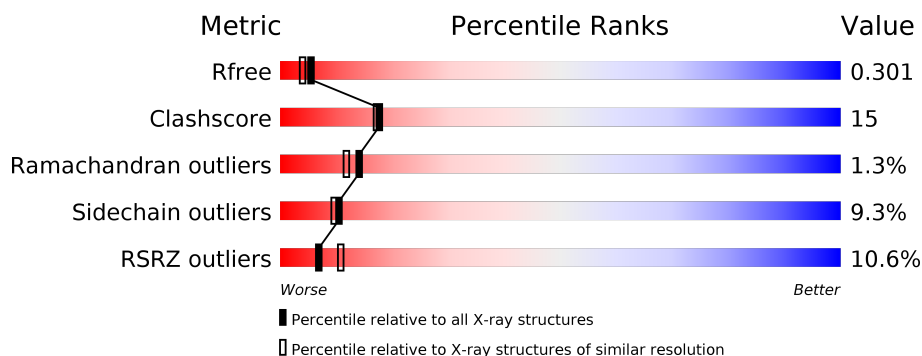
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.34 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}	100719	1570 (2.36-2.32)
Clashscore	112137	1673 (2.36-2.32)
Ramachandran outliers	110173	1654 (2.36-2.32)
Sidechain outliers	110143	1655 (2.36-2.32)
RSRZ outliers	101464	1576 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C	312	
1	E	312	
1	F	312	
1	G	312	
1	K	312	
1	M	312	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	C	301	-	-	-	X

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 (three-letter code: 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		

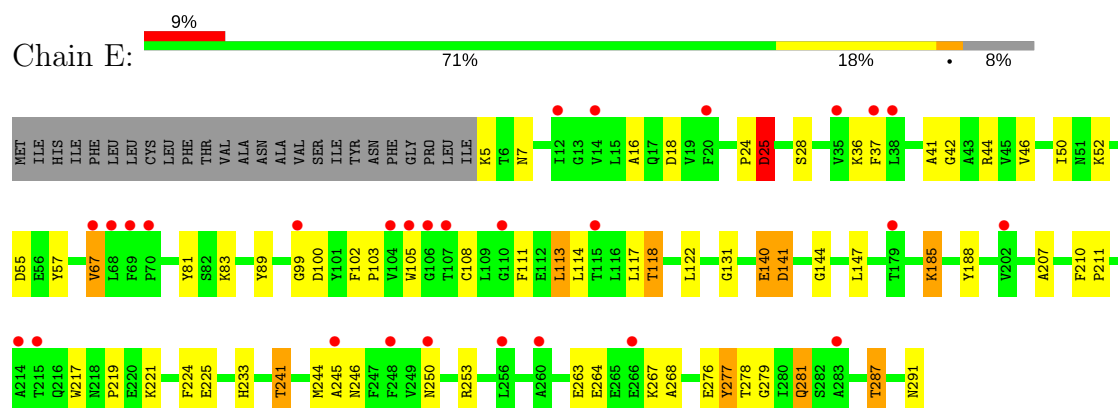
- Molecule 3 is water.

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		

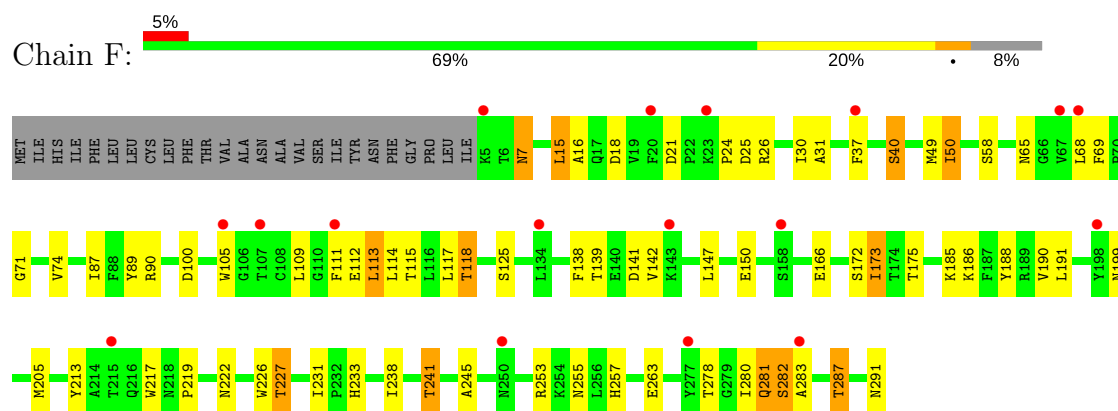
3 Residue-property plots

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

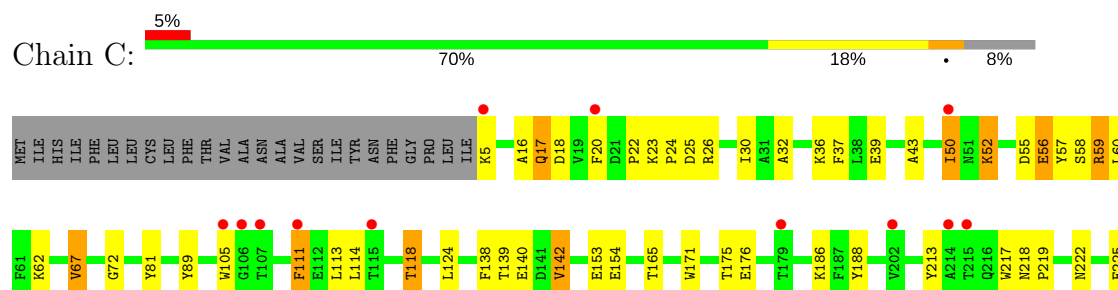
• Molecule 1: Gamma-glutamyl hydrolase



• Molecule 1: Gamma-glutamyl hydrolase

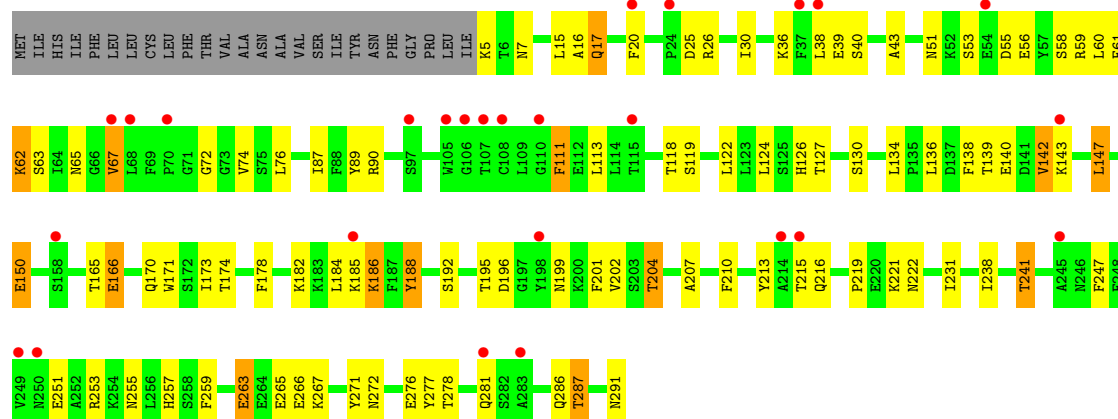


• Molecule 1: Gamma-glutamyl hydrolase

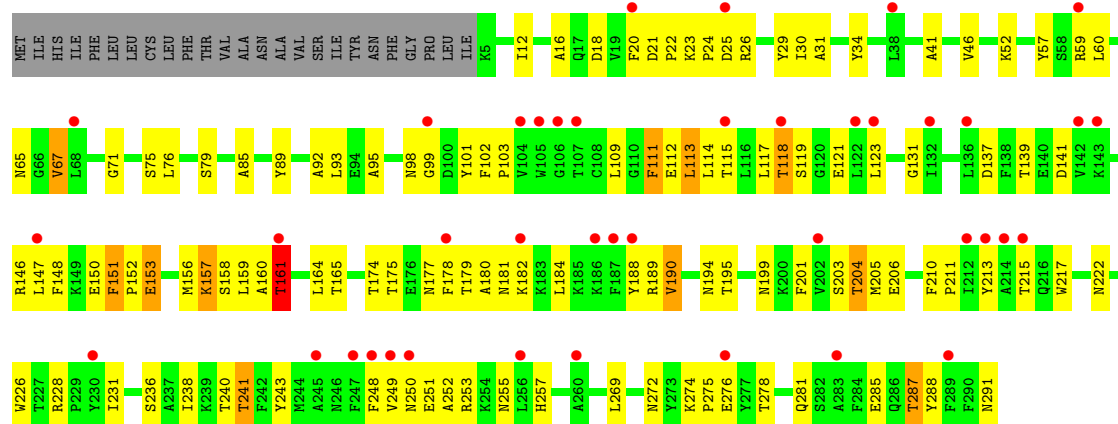




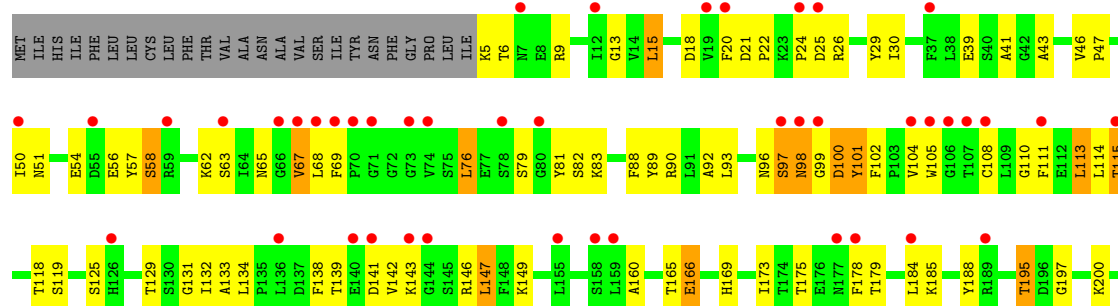
• Molecule 1: Gamma-glutamyl hydrolase

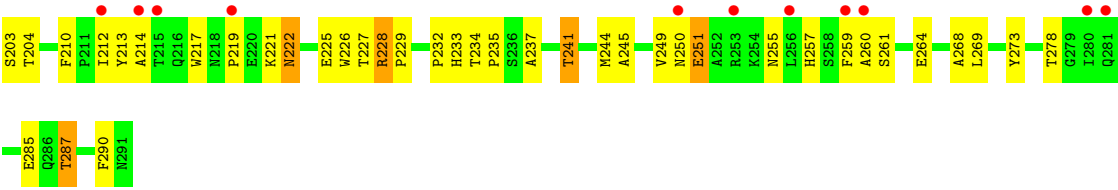


• Molecule 1: Gamma-glutamyl hydrolase



• 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) 98.2 (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 0.239 , 0.301	Depositor DCC
R_{free} test set	4413 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	43.5	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 38.3	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	1.08	2/2371 (0.1%)	0.91	4/3217 (0.1%)
1	E	0.90	2/2371 (0.1%)	0.85	3/3217 (0.1%)
1	F	0.92	1/2371 (0.0%)	0.83	0/3217
1	G	0.97	2/2371 (0.1%)	0.86	2/3217 (0.1%)
1	K	0.73	0/2371	0.71	0/3217
1	M	0.75	0/2371	0.76	0/3217
All	All	0.90	7/14226 (0.0%)	0.82	9/19302 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	2
1	M	0	1
All	All	0	3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	25	ASP	C-N	7.65	1.51	1.34
1	E	291	ASN	C-OXT	-6.12	1.11	1.23
1	G	150	GLU	CG-CD	5.35	1.59	1.51
1	F	150	GLU	CG-CD	5.28	1.59	1.51
1	C	153	GLU	CG-CD	5.22	1.59	1.51
1	G	188	TYR	CD2-CE2	-5.09	1.31	1.39
1	C	57	TYR	CD2-CE2	5.06	1.47	1.39

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	25	ASP	O-C-N	-10.59	105.76	122.70
1	E	25	ASP	C-N-CA	8.95	144.07	121.70
1	C	55	ASP	CB-CG-OD1	6.48	124.13	118.30
1	G	67	VAL	CB-CA-C	-6.43	99.18	111.40
1	E	25	ASP	CA-C-N	6.41	131.30	117.20
1	C	67	VAL	CB-CA-C	-6.02	99.97	111.40
1	G	238	ILE	CG1-CB-CG2	-5.91	98.41	111.40
1	C	52	LYS	CD-CE-NZ	-5.39	99.31	111.70
1	C	50	ILE	C-N-CA	-5.01	109.19	121.70

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	50	0
1	E	2307	0	2228	51	0
1	F	2307	0	2228	60	0
1	G	2307	0	2228	78	0
1	K	2307	0	2228	86	0
1	M	2307	0	2228	105	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	418	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 15.

All (418) 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:OE2	1:E:140:GLU:HA	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:G:65:ASN:HD22	1:G:255:ASN:HD22	1.27	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:111:PHE:CD2	1:K:111:PHE:C	2.57	0.77
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:F:255:ASN:HD21	1:F:257:HIS:CG	2.07	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:THR:HG21	1:C:188:TYR:OH	1.90	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: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: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:K:121:GLU:C	3:K:407:HOH:O	2.31	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: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
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:54:GLU:CD	1:M:90:ARG:HH22	1.98	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:K:111:PHE:HD2	1:K:111:PHE:C	1.99	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:F:68:LEU:C	1:F:68:LEU:HD23	2.18	0.64
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:18:ASP:CG	1:F:50:ILE:HD11	2.19	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:M:67:VAL:HG22	1:M:102:PHE:CE2	2.33	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:140:GLU:OE2	1:E:140:GLU:CA	2.39	0.61
1:E:44:ARG:HD3	1:F:226:TRP:CD1	2.35	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
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: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: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:F:49:MET:CE	1:F:49:MET:HA	2.33	0.58
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: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:C:50:ILE:HD11	1:C:81:TYR:HA	1.84	0.58
1:F:24:PRO:C	1:F:26:ARG:H	2.07	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:26:ARG:NH2	1:C:276:GLU:OE1	2.34	0.57
1:E:50:ILE:O	1:E:57:TYR:OH	2.21	0.57
1:C:285:GLU:HG3	1:G:271:TYR:CE1	2.39	0.57
1:M:195:THR:HG23	1:M:197:GLY:H	1.70	0.56
1:K:189:ARG:HG2	1:K:190:VAL:H	1.70	0.56
1:C:140:GLU:HG3	3:C:415:HOH:O	2.05	0.56
1:F:100:ASP:OD2	1:F:257:HIS:NE2	2.35	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
1:K:118:THR:HG21	1:K:188:TYR:OH	2.06	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:M:249:VAL:C	1:M:251:GLU:H	2.10	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:K:178:PHE:C	1:K:180:ALA:H	2.09	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: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:M:96:ASN:C	1:M:98:ASN:H	2.11	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:G:26:ARG:HH21	1:G:276:GLU:CD	2.11	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:K:178:PHE:C	1:K:180:ALA:N	2.62	0.53
1:M:115:THR:CA	1:M:184:LEU:HD21	2.36	0.53
1:M:111:PHE:CD1	1:M:214:ALA:HB1	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:F:25:ASP:H	1:F:291:ASN:ND2	1.94	0.52
1:E:253:ARG:NH2	1:F:238:ILE:HD12	2.25	0.52
1:F:173:ILE:O	1:F:173:ILE:HG12	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:146:ARG:NH2	1:M:210:PHE:O	2.42	0.51
1:M:98:ASN:O	1:M:100:ASP:N	2.43	0.51
1:C:218:ASN:ND2	3:C:419:HOH:O	2.43	0.51
1:F:278:THR:OG1	1:F:287:THR:CG2	2.58	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:108:CYS:O	1:M:111:PHE:HB3	2.12	0.49
1:E:105:TRP:HH2	1:E:244:MET:HE3	1.76	0.49
1:F:114:LEU:O	1:F:118:THR:HG23	2.13	0.49
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:243:TYR:HD2	3:K:401:HOH:O	1.96	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: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: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: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:HA	1:C:225:GLU:OE2	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:139:THR:HB	1:K:141:ASP:H	1.78	0.48
1:K:93:LEU:HA	1:K:210:PHE:HE1	1.79	0.48
1:C:111:PHE:C	1:C:111:PHE:CD2	2.88	0.48
1:C:228:ARG:HG3	1:C:230:TYR:OH	2.13	0.47
1:F:255:ASN:HD21	1:F:257:HIS:CB	2.26	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: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: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:F:118:THR:HG21	1:F:188:TYR:CZ	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:F:111:PHE:HE1	1:F:205:MET:HG2	1.79	0.47
1:F:24:PRO:C	1:F:26:ARG:N	2.68	0.47
1:F:105:TRP:CE3	1:F:213:TYR:HB2	2.50	0.47
1:E:141:ASP:OD1	1:E:141:ASP:N	2.44	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:E:225:GLU:O	1:E:233:HIS:HE1	1.98	0.47
1:E:100:ASP:C	1:E:100:ASP:OD1	2.52	0.47
1:E:278:THR:HG21	1:E:287:THR:HG23	1.97	0.47
1:M:129:THR:OG1	1:M:169:HIS:O	2.23	0.47
1:C:250:ASN:ND2	1:C:253:ARG:NH1	2.62	0.46
1:E:253:ARG:HH22	1:F:238:ILE:HD13	1.80	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:G:219:PRO:O	1:G:241:THR:HB	2.15	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:G:213:TYR:OH	1:G:251:GLU:OE2	2.27	0.46
1:M:76:LEU:HD23	1:M:76:LEU:N	2.31	0.46
1:C:285:GLU:OE2	1:C:285:GLU:HA	2.13	0.46
1:E:253:ARG:NH2	1:F:238:ILE:HD13	2.31	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:G:111:PHE:C	1:G:111:PHE:CD2	2.89	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:C:20:PHE:C	1:C:22:PRO:HD3	2.36	0.46
1:C:285:GLU:HG3	1:G:271:TYR:CZ	2.51	0.46
1:F:30:ILE:HG22	1:F:31:ALA:O	2.16	0.46
1:M:68:LEU:HA	1:M:105:TRP:O	2.16	0.46
1:C:52:LYS:HA	1:C:52:LYS:HD3	1.68	0.46
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:M:111:PHE:CD2	1:M:111:PHE:C	2.90	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: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:278:THR:CG2	1:M:287:THR:HG23	2.47	0.45
1:M:46:VAL:HA	1:M:47:PRO:HD2	1.76	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:166:GLU:CD	1:G:221:LYS:HD2	2.38	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:E:105:TRP:CH2	1:E:244:MET:HE3	2.53	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: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:G:36:LYS:HZ1	1:G:286:GLN:NE2	2.16	0.44
1:C:22:PRO:O	1:C:23:LYS:HG3	2.18	0.44
1:E:7:ASN:O	1:E:253:ARG:HG2	2.17	0.44
1:E:278:THR:OG1	1:E:287:THR:HG23	2.18	0.44
1:M:269:LEU:HD23	1:M:269:LEU:HA	1.82	0.44
1:K:146:ARG:HH11	1:K:146:ARG:HG3	1.82	0.44
1:K:152:PRO:O	1:K:153:GLU:C	2.56	0.43
1:K:165:THR:HB	1:K:217:TRP:CD2	2.53	0.43
1:K:21:ASP:HA	1:K:22:PRO:HD2	1.86	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG2	1:G:263:GLU:H	1.67	0.43
1:M:105:TRP:HH2	1:M:244:MET:HE3	1.82	0.43
1:M:217:TRP:CZ3	1:M:219:PRO:HB3	2.54	0.43
1:C:118:THR:HG21	1:C:188:TYR:CZ	2.52	0.43
1:C:105:TRP:CE3	1:C:213:TYR:HB2	2.54	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:M:132:ILE:CG1	1:M:133:ALA:N	2.81	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: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: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:222:ASN:HB2	1:C:241:THR:HG22	1.97	0.43
1:C:37:PHE:CE2	1:C:245:ALA:HB2	2.53	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:194:ASN:HB2	1:K:201:PHE:CZ	2.54	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:M:142:VAL:HG23	1:M:143:LYS:HD2	2.01	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:M:226:TRP:HB2	1:M:285:GLU:OE1	2.19	0.42
1:E:89:TYR:CZ	1:E:118:THR:HG22	2.52	0.42
1:G:147:LEU:HD23	1:G:247:PHE:CD2	2.54	0.42
1:E:185:LYS:HG3	1:E:185:LYS:O	2.20	0.42
1:E:89:TYR:OH	1:E:118:THR:CG2	2.64	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:146:ARG:HB2	1:K:206:GLU:OE1	2.20	0.42
1:K:24:PRO:O	1:K:25:ASP:CB	2.57	0.42
1:K:23:LYS:O	1:K:26:ARG:HB2	2.19	0.42
1:M:81:TYR:CE2	1:M:113:LEU:HD11	2.54	0.42
1:E:250:ASN:HA	1:E:250:ASN:HD22	1.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:111:PHE:CD2	1:F:111:PHE:C	2.93	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:136:LEU:HG	1:G:165:THR:HG21	2.02	0.41
1:G:56:GLU:HA	1:G:59:ARG:NH2	2.34	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:C:228:ARG:HB3	1:C:230:TYR:CE2	2.55	0.41
1:K:52:LYS:HB2	1:K:57:TYR:CZ	2.55	0.41
1:M:21:ASP:O	1:M:22:PRO:C	2.59	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:G:186:LYS:C	1:G:186:LYS:HD3	2.41	0.41
1:C:56:GLU:OE2	1:C:56:GLU:HA	2.20	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:M:178:PHE:O	1:M:179:THR:C	2.58	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: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:K:92:ALA:O	1:K:95:ALA:HB3	2.21	0.41
1:G:89:TYR:HH	1:G:118:THR:HG22	1.76	0.41
1:K:113:LEU:HD22	1:K:117:LEU:HG	2.02	0.41
1:K:12:ILE:HD11	1:K:252:ALA:HB2	2.02	0.41
1:M:227:THR:O	1:M:228:ARG:CD	2.68	0.41
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:G:61:PHE:CD2	1:G:61:PHE:C	2.94	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:M:56:GLU:C	1:M:58:SER:H	2.24	0.41
1:E:103:PRO:HA	1:E:211:PRO:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:52:LYS:HB2	1:E:57:TYR:CZ	2.56	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:G:25:ASP:H	1:G:291:ASN:HD22	1.70	0.40
1:M:259:PHE:O	1:M:260:ALA:C	2.59	0.40
1:F:282:SER:OG	1:F:283:ALA:N	2.53	0.40
1:K:213:TYR:N	1:K:213:TYR:CD1	2.89	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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	285/312 (91%)	271 (95%)	13 (5%)	1 (0%)	38	42
1	E	285/312 (91%)	264 (93%)	19 (7%)	2 (1%)	25	26
1	F	285/312 (91%)	270 (95%)	15 (5%)	0	100	100
1	G	285/312 (91%)	261 (92%)	23 (8%)	1 (0%)	38	42
1	K	285/312 (91%)	239 (84%)	36 (13%)	10 (4%)	4	2
1	M	285/312 (91%)	244 (86%)	33 (12%)	8 (3%)	6	3
All	All	1710/1872 (91%)	1549 (91%)	139 (8%)	22 (1%)	14	12

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	158	SER

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Mol	Chain	Res	Type
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%)	230 (92%)	20 (8%)	14	15
1	E	250/272 (92%)	232 (93%)	18 (7%)	17	17
1	F	250/272 (92%)	226 (90%)	24 (10%)	10	9
1	G	250/272 (92%)	220 (88%)	30 (12%)	6	5
1	K	250/272 (92%)	231 (92%)	19 (8%)	15	16
1	M	250/272 (92%)	222 (89%)	28 (11%)	7	6
All	All	1500/1632 (92%)	1361 (91%)	139 (9%)	10	9

All (139) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	5	LYS
1	E	18	ASP
1	E	55	ASP
1	E	67	VAL
1	E	83	LYS
1	E	113	LEU
1	E	118	THR
1	E	122	LEU
1	E	140	GLU
1	E	141	ASP
1	E	147	LEU
1	E	185	LYS
1	E	241	THR
1	E	264	GLU
1	E	276	GLU
1	E	277	TYR
1	E	281	GLN
1	E	287	THR
1	F	7	ASN
1	F	15	LEU
1	F	21	ASP
1	F	40	SER
1	F	50	ILE
1	F	58	SER
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	185	LYS
1	F	186	LYS
1	F	217	TRP
1	F	227	THR
1	F	241	THR
1	F	281	GLN
1	F	282	SER
1	F	287	THR

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Mol	Chain	Res	Type
1	C	5	LYS
1	C	17	GLN
1	C	18	ASP
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	154	GLU
1	C	175	THR
1	C	176	GLU
1	C	186	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
1	G	17	GLN
1	G	20	PHE
1	G	40	SER
1	G	62	LYS
1	G	63	SER
1	G	67	VAL
1	G	74	VAL
1	G	76	LEU
1	G	111	PHE
1	G	113	LEU
1	G	119	SER
1	G	127	THR
1	G	130	SER
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

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Mol	Chain	Res	Type
1	G	185	LYS
1	G	186	LYS
1	G	204	THR
1	G	241	THR
1	G	263	GLU
1	G	267	LYS
1	G	277	TYR
1	G	287	THR
1	K	18	ASP
1	K	20	PHE
1	K	59	ARG
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	151	PHE
1	K	161	THR
1	K	190	VAL
1	K	203	SER
1	K	204	THR
1	K	241	THR
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	101	TYR
1	M	113	LEU
1	M	125	SER

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Mol	Chain	Res	Type
1	M	147	LEU
1	M	149	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	241	THR
1	M	251	GLU
1	M	287	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	167	ASN
1	E	218	ASN
1	E	250	ASN
1	F	51	ASN
1	F	167	ASN
1	F	216	GLN
1	F	218	ASN
1	F	255	ASN
1	F	272	ASN
1	F	281	GLN
1	F	286	GLN
1	F	291	ASN
1	C	167	ASN
1	C	177	ASN
1	C	218	ASN
1	C	250	ASN
1	G	126	HIS
1	G	128	ASN
1	G	167	ASN
1	G	255	ASN
1	G	272	ASN
1	G	286	GLN
1	G	291	ASN
1	K	181	ASN
1	K	218	ASN

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Mol	Chain	Res	Type
1	K	233	HIS
1	K	250	ASN
1	M	96	ASN
1	M	128	ASN
1	M	167	ASN
1	M	216	GLN
1	M	222	ASN
1	M	246	ASN
1	M	255	ASN
1	M	257	HIS
1	M	286	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	C	301	-	5,5,5	0.71	0	5,5,5	0.56	0
2	GOL	G	301	-	5,5,5	0.53	0	5,5,5	0.27	0
2	GOL	K	301	-	5,5,5	0.57	0	5,5,5	0.51	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	C	301	-	-	0/4/4/4	0/0/0/0
2	GOL	G	301	-	-	0/4/4/4	0/0/0/0
2	GOL	K	301	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	0.17	16 (5%)	25 35	18, 34, 51, 67	9 (3%)
1	E	287/312 (91%)	0.44	28 (9%)	8 13	26, 43, 60, 68	9 (3%)
1	F	287/312 (91%)	0.29	17 (5%)	23 33	27, 45, 62, 74	5 (1%)
1	G	287/312 (91%)	0.49	26 (9%)	10 15	23, 45, 62, 69	5 (1%)
1	K	287/312 (91%)	0.93	41 (14%)	3 5	38, 63, 80, 87	9 (3%)
1	M	287/312 (91%)	1.18	55 (19%)	1 2	35, 66, 87, 99	5 (1%)
All	All	1722/1872 (91%)	0.58	183 (10%)	7 11	18, 49, 77, 99	42 (2%)

All (183) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	144	GLY	7.2
1	M	280	ILE	6.9
1	K	250	ASN	6.2
1	M	250	ASN	6.1
1	E	68	LEU	5.4
1	K	20	PHE	5.3
1	F	198	TYR	5.2
1	G	250	ASN	5.2
1	M	20	PHE	5.2
1	K	178	PHE	5.1
1	M	59	ARG	4.7
1	C	20	PHE	4.5
1	M	97	SER	4.3
1	M	105	TRP	4.2
1	M	67	VAL	4.2
1	M	24	PRO	4.2
1	C	202	VAL	4.2
1	C	115	THR	4.1
1	M	107	THR	4.1

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Mol	Chain	Res	Type	RSRZ
1	E	20	PHE	4.1
1	M	215	THR	4.0
1	G	245	ALA	4.0
1	E	250	ASN	4.0
1	M	111	PHE	3.9
1	F	250	ASN	3.9
1	M	108	CYS	3.8
1	E	115	THR	3.8
1	E	107	THR	3.7
1	K	202	VAL	3.7
1	M	74	VAL	3.7
1	M	214	ALA	3.7
1	E	105	TRP	3.7
1	M	126	HIS	3.7
1	K	182	LYS	3.6
1	K	245	ALA	3.6
1	E	283	ALA	3.5
1	E	106	GLY	3.5
1	K	105	TRP	3.4
1	K	25	ASP	3.4
1	M	68	LEU	3.3
1	M	155	LEU	3.3
1	M	69	PHE	3.3
1	C	250	ASN	3.3
1	K	249	VAL	3.3
1	F	20	PHE	3.2
1	K	248	PHE	3.2
1	M	98	ASN	3.2
1	G	105	TRP	3.2
1	M	104	VAL	3.2
1	K	59	ARG	3.2
1	G	283	ALA	3.2
1	M	99	GLY	3.2
1	K	104	VAL	3.1
1	E	215	THR	3.1
1	G	107	THR	3.1
1	G	115	THR	3.1
1	M	178	PHE	3.1
1	K	276	GLU	3.1
1	E	179	THR	3.1
1	M	106	GLY	3.1
1	E	14	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	M	25	ASP	3.0
1	M	143	LYS	3.0
1	E	70	PRO	3.0
1	M	219	PRO	3.0
1	G	68	LEU	3.0
1	K	283	ALA	3.0
1	K	99	GLY	3.0
1	F	68	LEU	2.9
1	K	186	LYS	2.9
1	M	12	ILE	2.8
1	F	107	THR	2.8
1	E	260	ALA	2.8
1	M	256	LEU	2.8
1	K	107	THR	2.8
1	M	115	THR	2.8
1	G	198	TYR	2.8
1	K	188	TYR	2.8
1	M	19	VAL	2.8
1	K	213	TYR	2.8
1	E	37	PHE	2.8
1	E	245	ALA	2.8
1	G	143	LYS	2.7
1	M	78	SER	2.7
1	E	69	PHE	2.7
1	E	266	GLU	2.7
1	M	7	ASN	2.7
1	C	50	ILE	2.7
1	M	259	PHE	2.7
1	C	106	GLY	2.7
1	G	281	GLN	2.7
1	C	214	ALA	2.6
1	K	260	ALA	2.6
1	E	202	VAL	2.6
1	G	97	SER	2.6
1	G	20	PHE	2.6
1	F	158	SER	2.6
1	C	107	THR	2.6
1	F	5	LYS	2.6
1	G	215	THR	2.5
1	M	184	LEU	2.5
1	F	37	PHE	2.5
1	M	140	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	K	68	LEU	2.5
1	K	122	LEU	2.5
1	E	35	VAL	2.5
1	M	260	ALA	2.5
1	C	281	GLN	2.5
1	K	247	PHE	2.4
1	K	106	GLY	2.4
1	K	123	LEU	2.4
1	K	136	LEU	2.4
1	K	215	THR	2.4
1	M	80	GLY	2.4
1	M	136	LEU	2.4
1	F	143	LYS	2.4
1	C	5	LYS	2.4
1	K	132	ILE	2.4
1	F	134	LEU	2.4
1	M	63	SER	2.4
1	C	280	ILE	2.4
1	M	158	SER	2.4
1	M	189	ARG	2.3
1	G	38	LEU	2.3
1	M	159	LEU	2.3
1	E	67	VAL	2.3
1	G	185	LYS	2.3
1	G	108	CYS	2.3
1	E	110	GLY	2.3
1	F	111	PHE	2.3
1	F	283	ALA	2.3
1	K	147	LEU	2.3
1	G	110	GLY	2.3
1	E	248	PHE	2.3
1	G	67	VAL	2.3
1	G	249	VAL	2.3
1	F	23	LYS	2.3
1	K	212	ILE	2.3
1	G	54	GLU	2.2
1	F	67	VAL	2.2
1	K	289	PHE	2.2
1	C	215	THR	2.2
1	E	99	GLY	2.2
1	K	214	ALA	2.2
1	K	38	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	M	281	GLN	2.2
1	K	230	TYR	2.2
1	G	70	PRO	2.2
1	M	55	ASP	2.2
1	M	73	GLY	2.2
1	M	50	ILE	2.2
1	E	38	LEU	2.2
1	M	71	GLY	2.2
1	G	37	PHE	2.1
1	C	245	ALA	2.1
1	K	143	LYS	2.1
1	E	12	ILE	2.1
1	G	158	SER	2.1
1	E	214	ALA	2.1
1	C	105	TRP	2.1
1	K	161	THR	2.1
1	F	277	TYR	2.1
1	M	37	PHE	2.1
1	M	66	GLY	2.1
1	M	70	PRO	2.1
1	K	256	LEU	2.1
1	M	212	ILE	2.1
1	M	253	ARG	2.1
1	E	104	VAL	2.1
1	K	142	VAL	2.1
1	E	256	LEU	2.0
1	K	115	THR	2.0
1	K	118	THR	2.0
1	G	106	GLY	2.0
1	F	105	TRP	2.0
1	F	215	THR	2.0
1	C	179	THR	2.0
1	G	24	PRO	2.0
1	C	111	PHE	2.0
1	K	187	PHE	2.0
1	M	177	ASN	2.0
1	M	141	ASP	2.0
1	G	214	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	GOL	C	301	6/6	0.72	0.29	3.84	62,69,70,70	0
2	GOL	G	301	6/6	0.88	0.24	1.70	55,59,59,60	0
2	GOL	K	301	6/6	0.81	0.19	-	66,67,67,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.