



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:05 PM UTC

PDB ID : 8IJ8 / pdb_00008ij8
Title : Crystal structure of alcohol dehydrogenase M4 mutant from Burkholderia gladioli
Authors : Han, X.; Mei, Z.L.; Liu, W.D.; Sun, Z.T.; Ma, J.A.
Deposited on : 2023-02-26
Resolution : 2.38 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

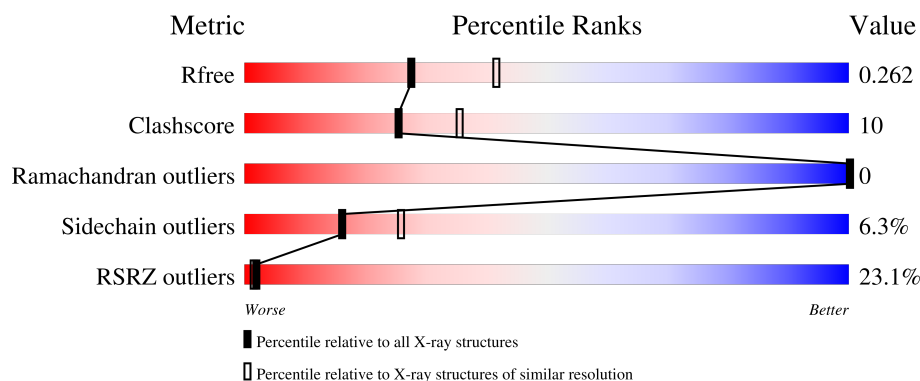
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.38 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	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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	251	
1	B	251	
1	C	251	
1	D	251	
1	E	251	

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Mol	Chain	Length	Quality of chain
1	F	251	19% 78% 20% ••
1	G	251	31% 76% 19% ••
1	H	251	66% 57% 36% • 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14566 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 Putative short-chain dehydrogenases/reductase family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			1806	1121	327	356	2			
1	B	250	Total	C	N	O	S	0	0	0
			1802	1118	326	356	2			
1	C	249	Total	C	N	O	S	0	0	0
			1786	1111	316	357	2			
1	D	249	Total	C	N	O	S	0	0	0
			1799	1118	323	356	2			
1	E	249	Total	C	N	O	S	0	0	0
			1790	1113	317	358	2			
1	F	249	Total	C	N	O	S	0	0	0
			1776	1105	317	352	2			
1	G	248	Total	C	N	O	S	0	0	0
			1754	1093	306	353	2			
1	H	239	Total	C	N	O	S	0	0	0
			1668	1046	286	334	2			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	84	ILE	VAL	engineered mutation	UNP F2LIG4
A	92	ALA	GLY	engineered mutation	UNP F2LIG4
A	140	LYS	ALA	engineered mutation	UNP F2LIG4
A	203	THR	LEU	engineered mutation	UNP F2LIG4
B	84	ILE	VAL	engineered mutation	UNP F2LIG4
B	92	ALA	GLY	engineered mutation	UNP F2LIG4
B	140	LYS	ALA	engineered mutation	UNP F2LIG4
B	203	THR	LEU	engineered mutation	UNP F2LIG4
C	84	ILE	VAL	engineered mutation	UNP F2LIG4
C	92	ALA	GLY	engineered mutation	UNP F2LIG4
C	140	LYS	ALA	engineered mutation	UNP F2LIG4
C	203	THR	LEU	engineered mutation	UNP F2LIG4
D	84	ILE	VAL	engineered mutation	UNP F2LIG4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	92	ALA	GLY	engineered mutation	UNP F2LIG4
D	140	LYS	ALA	engineered mutation	UNP F2LIG4
D	203	THR	LEU	engineered mutation	UNP F2LIG4
E	84	ILE	VAL	engineered mutation	UNP F2LIG4
E	92	ALA	GLY	engineered mutation	UNP F2LIG4
E	140	LYS	ALA	engineered mutation	UNP F2LIG4
E	203	THR	LEU	engineered mutation	UNP F2LIG4
F	84	ILE	VAL	engineered mutation	UNP F2LIG4
F	92	ALA	GLY	engineered mutation	UNP F2LIG4
F	140	LYS	ALA	engineered mutation	UNP F2LIG4
F	203	THR	LEU	engineered mutation	UNP F2LIG4
G	84	ILE	VAL	engineered mutation	UNP F2LIG4
G	92	ALA	GLY	engineered mutation	UNP F2LIG4
G	140	LYS	ALA	engineered mutation	UNP F2LIG4
G	203	THR	LEU	engineered mutation	UNP F2LIG4
H	84	ILE	VAL	engineered mutation	UNP F2LIG4
H	92	ALA	GLY	engineered mutation	UNP F2LIG4
H	140	LYS	ALA	engineered mutation	UNP F2LIG4
H	203	THR	LEU	engineered mutation	UNP F2LIG4

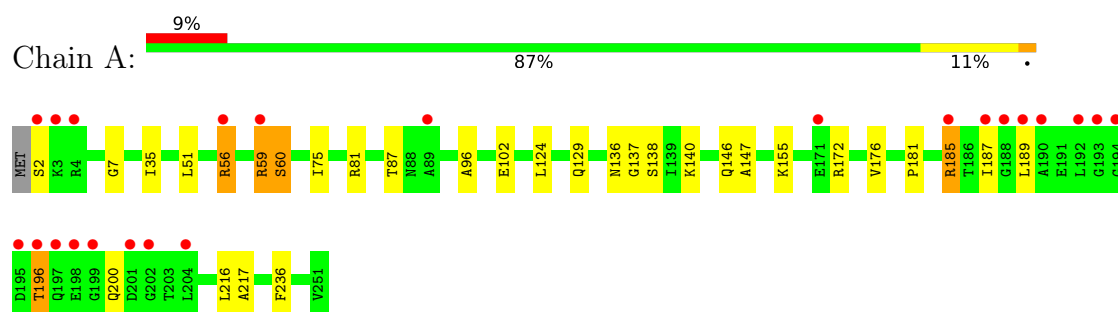
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	79	Total O 79 79	0	0
2	B	76	Total O 76 76	0	0
2	C	48	Total O 48 48	0	0
2	D	46	Total O 46 46	0	0
2	E	48	Total O 48 48	0	0
2	F	39	Total O 39 39	0	0
2	G	33	Total O 33 33	0	0
2	H	16	Total O 16 16	0	0

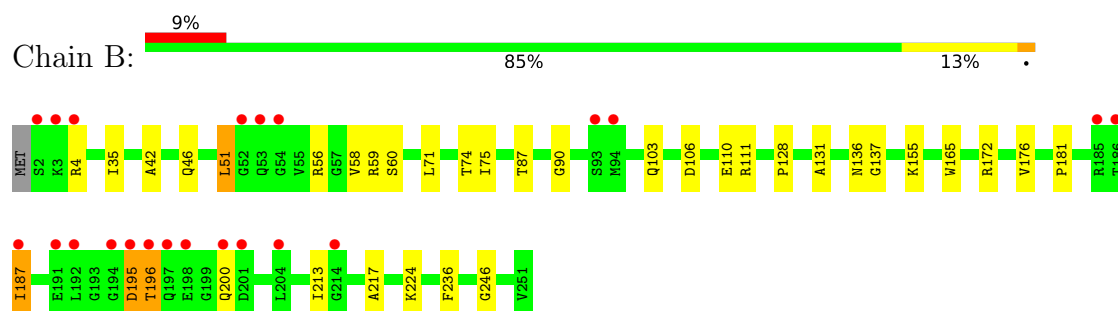
3 Residue-property plots [i](#)

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.

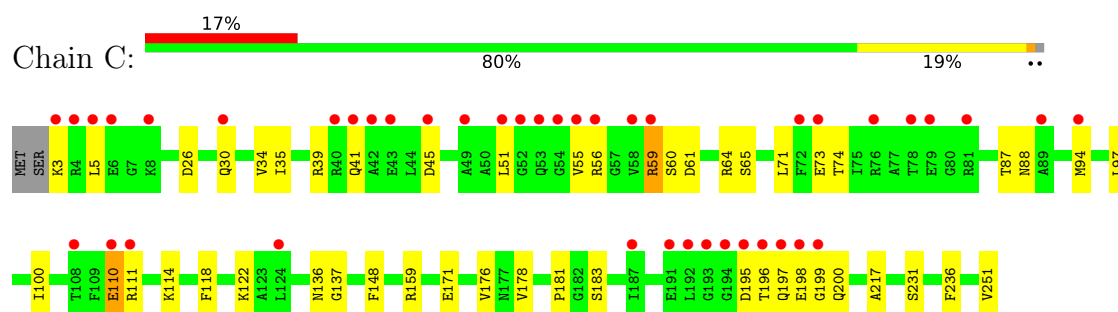
- Molecule 1: Putative short-chain dehydrogenases/reductase family protein



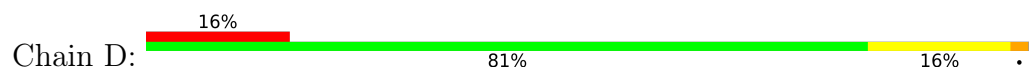
- Molecule 1: Putative short-chain dehydrogenases/reductase family protein

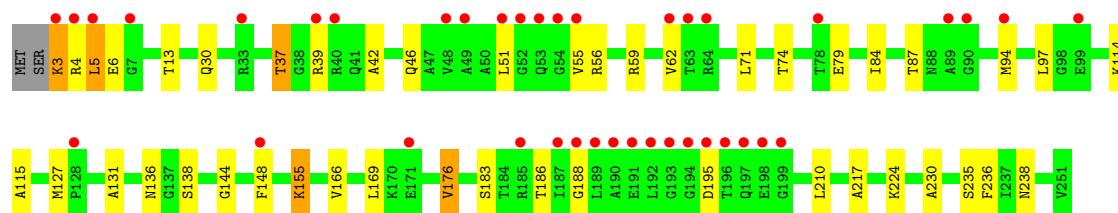


- Molecule 1: Putative short-chain dehydrogenases/reductase family protein

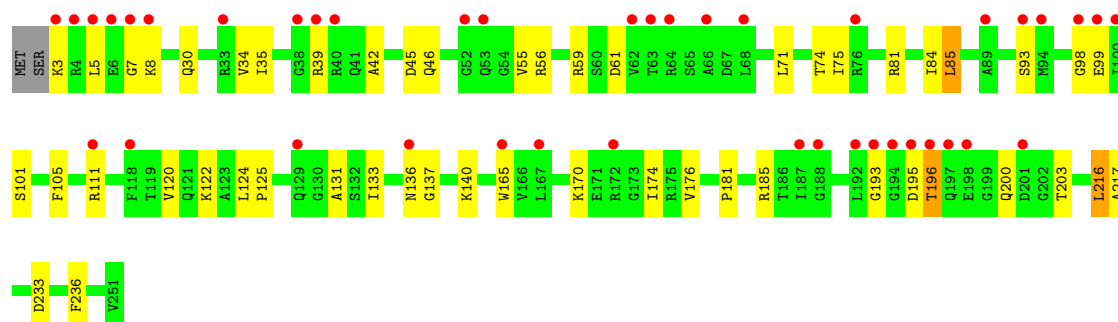
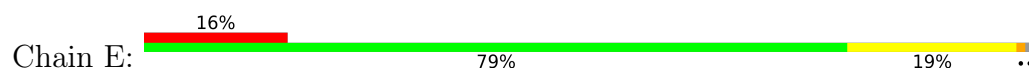


- Molecule 1: Putative short-chain dehydrogenases/reductase family protein

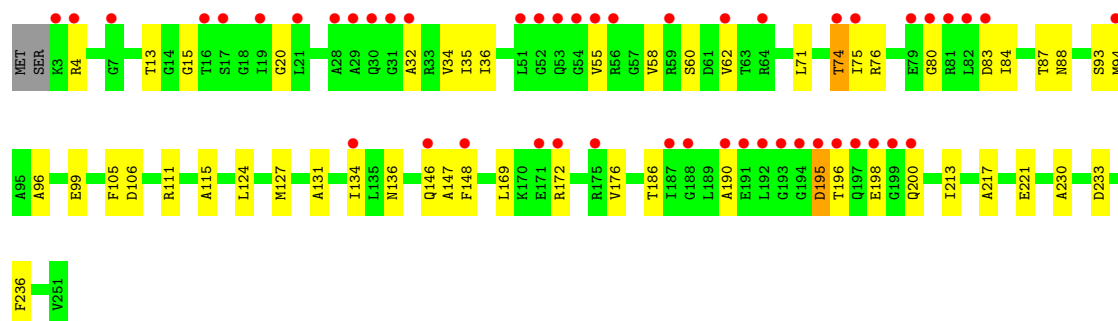
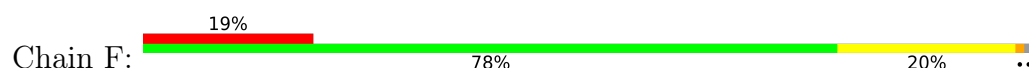




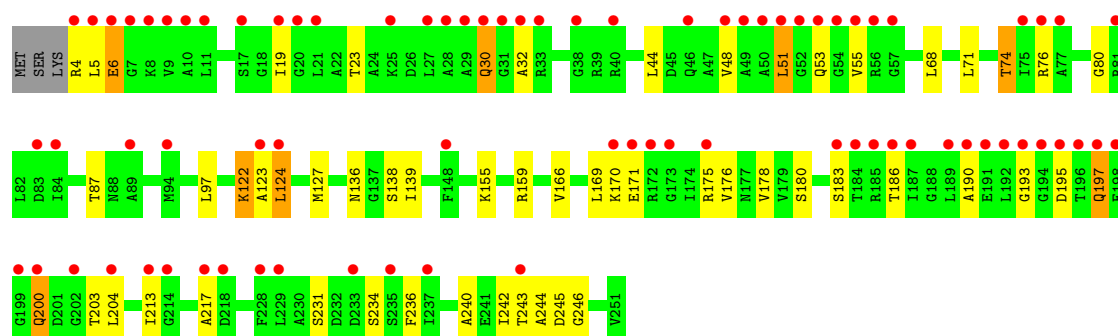
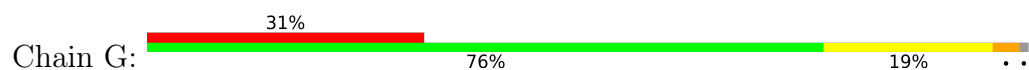
- Molecule 1: Putative short-chain dehydrogenases/reductase family protein



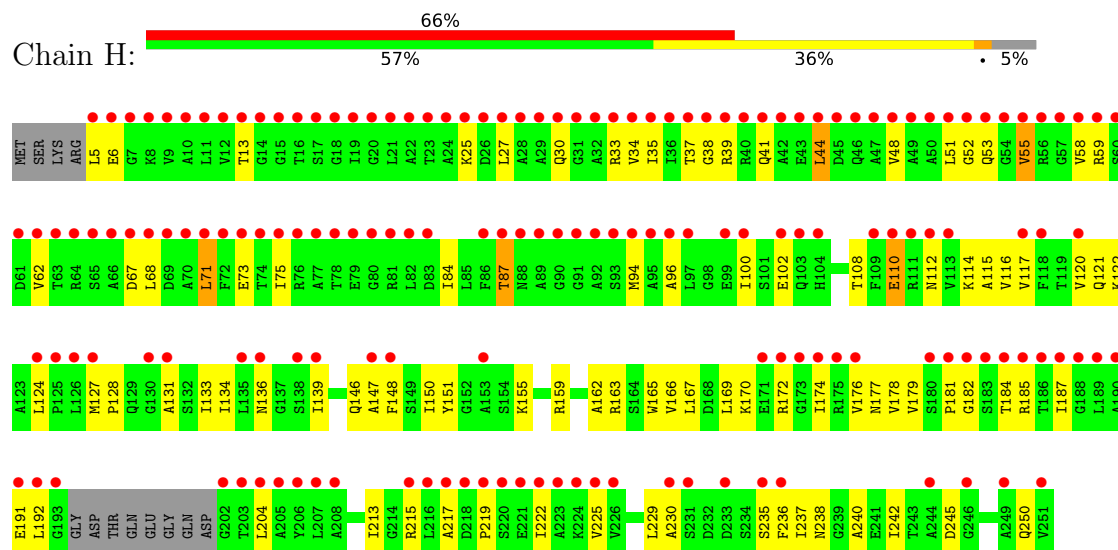
- Molecule 1: Putative short-chain dehydrogenases/reductase family protein



- Molecule 1: Putative short-chain dehydrogenases/reductase family protein



Chain H:



4 Data and refinement statistics

Property	Value	Source
Space group	P 4	Depositor
Cell constants a, b, c, α , β , γ	141.31Å 141.31Å 164.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.96 – 2.38 49.96 – 2.38	Depositor EDS
% Data completeness (in resolution range)	98.0 (49.96-2.38) 97.9 (49.96-2.38)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 2.37Å)	Xtriage
Refinement program	PHENIX 1.1932-4158	Depositor
R, R_{free}	0.225 , 0.258 0.233 , 0.262	Depositor DCC
R_{free} test set	6315 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	41.4	Xtriage
Anisotropy	0.487	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 46.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.048 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14566	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.35% 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	0.40	0/1823	0.65	0/2465
1	B	0.36	0/1819	0.62	1/2461 (0.0%)
1	C	0.46	0/1803	0.75	0/2441
1	D	0.43	0/1816	0.68	2/2456 (0.1%)
1	E	0.42	0/1807	0.66	0/2446
1	F	0.49	0/1793	0.77	1/2429 (0.0%)
1	G	0.50	0/1771	0.79	3/2402 (0.1%)
1	H	0.46	0/1684	0.80	4/2289 (0.2%)
All	All	0.44	0/14316	0.72	11/19389 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	195	ASP	CB-CA-C	-5.46	102.27	110.90
1	D	195	ASP	N-CA-C	5.42	117.00	111.14
1	B	103	GLN	CA-CB-CG	-5.39	103.32	114.10
1	H	33	ARG	CA-C-N	-5.35	115.55	122.99
1	H	33	ARG	C-N-CA	-5.35	115.55	122.99
1	G	246	GLY	N-CA-C	-5.16	108.12	115.30
1	G	197	GLN	CA-C-N	-5.16	114.39	122.65
1	G	197	GLN	C-N-CA	-5.16	114.39	122.65
1	F	83	ASP	N-CA-C	-5.08	107.63	113.88
1	H	110	GLU	CB-CG-CD	-5.06	104.00	112.60
1	H	110	GLU	CA-CB-CG	5.06	124.21	114.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1806	0	1838	37	0
1	B	1802	0	1827	24	0
1	C	1786	0	1802	34	0
1	D	1799	0	1828	35	0
1	E	1790	0	1808	39	0
1	F	1776	0	1788	38	0
1	G	1754	0	1749	38	0
1	H	1668	0	1658	66	0
2	A	79	0	0	4	0
2	B	76	0	0	1	0
2	C	48	0	0	1	0
2	D	46	0	0	1	0
2	E	48	0	0	2	0
2	F	39	0	0	4	0
2	G	33	0	0	1	0
2	H	16	0	0	3	0
All	All	14566	0	14298	273	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 10.

All (273) 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:A:59:ARG:HG2	1:A:59:ARG:HH11	1.13	1.10
1:E:39:ARG:HD3	1:E:111:ARG:NH2	1.70	1.05
1:A:185:ARG:HG3	1:A:185:ARG:NH1	1.67	1.03
1:A:185:ARG:HG3	1:A:185:ARG:HH11	0.86	1.01
1:A:185:ARG:HH11	1:A:185:ARG:CG	1.77	0.93
1:D:84:ILE:HD13	1:D:230:ALA:HB1	1.51	0.90
1:E:39:ARG:HD3	1:E:111:ARG:HH22	1.41	0.86
1:A:56:ARG:HH22	1:A:75:ILE:CG1	1.90	0.85
1:E:39:ARG:HD3	1:E:111:ARG:CZ	2.09	0.83
1:A:185:ARG:HH12	1:A:216:LEU:HD12	1.42	0.82
1:A:59:ARG:HG2	1:A:59:ARG:NH1	1.83	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:ARG:NH2	1:A:75:ILE:CG1	2.44	0.80
1:A:185:ARG:NH1	1:A:216:LEU:HD12	1.95	0.80
1:B:56:ARG:HH22	1:B:74:THR:HG23	1.46	0.79
1:B:71:LEU:O	1:B:74:THR:HG22	1.83	0.78
1:G:213:ILE:HD11	1:H:238:ASN:HD22	1.49	0.78
1:F:172:ARG:HD3	2:F:315:HOH:O	1.83	0.76
1:A:56:ARG:NH2	1:A:75:ILE:HG13	2.01	0.75
1:G:5:LEU:HB2	1:G:30:GLN:HB3	1.69	0.75
1:A:56:ARG:HH22	1:A:75:ILE:HG13	1.52	0.74
1:B:195:ASP:OD1	1:B:195:ASP:N	2.16	0.74
1:G:180:SER:HB2	1:G:243:THR:HG22	1.70	0.73
1:A:7:GLY:O	1:A:81:ARG:NH2	2.21	0.73
1:A:56:ARG:NH2	1:A:75:ILE:HG12	2.03	0.73
1:C:61:ASP:HB3	1:C:64:ARG:HD2	1.70	0.72
1:G:175:ARG:NH1	1:G:234:SER:O	2.22	0.71
1:E:30:GLN:NE2	2:E:301:HOH:O	2.23	0.71
1:A:35:ILE:HG12	1:A:56:ARG:NE	2.07	0.69
1:F:87:THR:O	1:F:136:ASN:HB2	1.92	0.68
1:G:175:ARG:HH12	1:G:234:SER:C	2.03	0.66
1:B:172:ARG:HG2	2:B:336:HOH:O	1.94	0.66
1:A:140:LYS:NZ	2:A:301:HOH:O	2.28	0.66
1:E:185:ARG:HG3	1:E:216:LEU:HD23	1.79	0.65
1:D:56:ARG:NH1	1:E:45:ASP:OD2	2.29	0.65
1:H:39:ARG:O	1:H:59:ARG:NH1	2.30	0.64
1:G:5:LEU:HB3	1:G:32:ALA:HB2	1.79	0.64
1:H:167:LEU:O	1:H:170:LYS:HG2	1.98	0.64
1:F:172:ARG:CZ	2:F:302:HOH:O	2.46	0.63
1:A:185:ARG:NH1	1:A:185:ARG:CG	2.46	0.63
1:H:187:ILE:O	1:H:191:GLU:HG3	1.99	0.62
1:H:34:VAL:HB	1:H:55:VAL:HG22	1.83	0.60
1:D:59:ARG:HH21	1:E:59:ARG:HH21	1.48	0.60
1:C:41:GLN:NE2	1:C:45:ASP:OD1	2.30	0.60
1:F:20:GLY:H	1:F:88:ASN:ND2	1.99	0.60
1:G:51:LEU:HD13	1:G:55:VAL:HG11	1.84	0.59
1:B:87:THR:O	1:B:136:ASN:HB2	2.03	0.59
1:D:51:LEU:HB3	1:D:55:VAL:HG21	1.84	0.59
1:G:51:LEU:HB3	1:G:55:VAL:HG21	1.84	0.59
1:H:100:ILE:HD13	1:H:150:ILE:HG12	1.83	0.59
1:H:185:ARG:O	1:H:219:PRO:HD3	2.02	0.59
1:G:236:PHE:CD2	1:H:217:ALA:HB2	2.38	0.59
1:H:117:VAL:HG12	1:H:165:TRP:CZ2	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:236:PHE:CE2	1:H:217:ALA:HB2	2.37	0.59
1:H:44:LEU:O	1:H:48:VAL:HG23	2.02	0.59
1:D:5:LEU:HB2	1:D:30:GLN:HB3	1.84	0.58
1:B:42:ALA:O	1:B:46:GLN:HG3	2.04	0.58
1:D:56:ARG:NH2	1:D:79:GLU:OE1	2.36	0.58
1:H:222:ILE:O	1:H:225:VAL:HG12	2.02	0.58
1:H:177:ASN:ND2	1:H:237:ILE:HG22	2.19	0.58
1:H:110:GLU:HA	1:H:114:LYS:HB3	1.87	0.57
1:H:151:TYR:O	1:H:155:LYS:HG2	2.05	0.57
1:E:39:ARG:HH11	1:E:111:ARG:NH1	2.01	0.56
1:D:13:THR:HA	1:D:37:THR:HB	1.86	0.56
1:C:110:GLU:HA	1:C:114:LYS:HB3	1.87	0.56
1:G:71:LEU:O	1:G:74:THR:HG22	2.06	0.56
1:E:7:GLY:O	1:E:81:ARG:NH2	2.38	0.56
1:F:96:ALA:O	1:F:99:GLU:HB2	2.06	0.56
1:E:136:ASN:HB2	2:E:310:HOH:O	2.06	0.56
1:C:97:LEU:HD23	1:F:169:LEU:HD21	1.87	0.55
1:E:39:ARG:HG2	1:E:61:ASP:HA	1.88	0.55
1:C:34:VAL:HB	1:C:55:VAL:HG22	1.89	0.55
1:A:102:GLU:HG3	1:D:114:LYS:HE3	1.87	0.55
1:E:196:THR:O	1:E:200:GLN:HG3	2.06	0.55
1:G:87:THR:O	1:G:136:ASN:HB2	2.07	0.55
1:H:5:LEU:HB2	1:H:30:GLN:HB3	1.89	0.55
1:H:177:ASN:ND2	1:H:240:ALA:H	2.05	0.55
1:G:193:GLY:HA2	1:G:203:THR:HG21	1.88	0.54
1:H:37:THR:HA	1:H:58:VAL:O	2.07	0.54
1:E:42:ALA:O	1:E:46:GLN:HG3	2.07	0.54
1:H:177:ASN:HD22	1:H:240:ALA:H	1.55	0.54
1:F:71:LEU:O	1:F:74:THR:HG22	2.08	0.54
1:G:138:SER:HB3	1:G:155:LYS:HG3	1.89	0.54
1:A:60:SER:HB3	2:A:332:HOH:O	2.07	0.54
1:C:87:THR:O	1:C:136:ASN:HB2	2.07	0.54
1:G:124:LEU:HD21	1:G:169:LEU:HD21	1.90	0.54
1:G:240:ALA:HA	1:H:250:GLN:HE21	1.72	0.54
1:F:124:LEU:HD13	1:F:172:ARG:NH1	2.23	0.53
1:C:196:THR:HG22	1:C:199:GLY:H	1.73	0.53
1:H:184:THR:HG22	1:H:217:ALA:HB3	1.90	0.53
1:E:5:LEU:HB2	1:E:30:GLN:HB3	1.89	0.53
1:H:184:THR:HG23	2:H:307:HOH:O	2.08	0.52
1:F:96:ALA:HA	1:F:147:ALA:HA	1.91	0.52
1:H:225:VAL:HG21	1:H:242:ILE:HG21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:62:VAL:HB	1:F:115:ALA:HB1	1.91	0.52
1:B:224:LYS:HB3	1:E:233:ASP:HB3	1.91	0.52
1:E:71:LEU:O	1:E:74:THR:HG22	2.10	0.52
1:E:120:VAL:HG21	1:E:165:TRP:HZ3	1.74	0.52
1:E:170:LYS:NZ	1:H:146:GLN:HE22	2.08	0.52
1:H:172:ARG:NE	2:H:304:HOH:O	2.37	0.52
1:B:58:VAL:HG21	1:B:74:THR:HG21	1.91	0.52
1:F:76:ARG:HA	1:F:80:GLY:HA2	1.91	0.52
1:G:68:LEU:HB3	1:G:122:LYS:HD3	1.91	0.52
1:C:94:MET:HB3	1:C:148:PHE:CZ	2.45	0.52
1:D:3:LYS:HD3	1:D:30:GLN:HA	1.91	0.52
1:H:128:PRO:HD2	1:H:131:ALA:HB2	1.91	0.52
1:D:155:LYS:NZ	2:D:303:HOH:O	2.43	0.52
1:D:236:PHE:CE2	1:F:217:ALA:HB2	2.45	0.52
1:F:58:VAL:HG21	1:F:74:THR:HG21	1.91	0.51
1:D:217:ALA:HB2	1:F:236:PHE:CD2	2.45	0.51
1:G:175:ARG:NH1	1:G:234:SER:C	2.65	0.51
1:H:38:GLY:N	1:H:44:LEU:HD13	2.26	0.51
1:D:127:MET:HE2	1:D:131:ALA:HB1	1.92	0.51
1:A:35:ILE:HG12	1:A:56:ARG:CZ	2.40	0.51
1:H:127:MET:HE2	1:H:131:ALA:HB1	1.92	0.51
1:E:195:ASP:OD1	1:E:195:ASP:N	2.43	0.51
1:H:117:VAL:HG12	1:H:165:TRP:HZ2	1.75	0.51
1:D:186:THR:HG22	1:D:188:GLY:H	1.76	0.51
1:E:39:ARG:HD3	1:E:111:ARG:NH1	2.25	0.51
1:F:35:ILE:HD13	1:F:75:ILE:HG12	1.93	0.51
1:F:172:ARG:NH2	2:F:302:HOH:O	2.44	0.51
1:H:136:ASN:ND2	2:H:302:HOH:O	2.35	0.50
1:C:114:LYS:HB2	1:F:105:PHE:CE2	2.46	0.50
1:A:136:ASN:ND2	2:A:302:HOH:O	2.29	0.50
1:B:236:PHE:CE2	1:E:217:ALA:HB2	2.47	0.50
1:H:25:LYS:HA	1:H:53:GLN:NE2	2.27	0.50
1:D:217:ALA:HB2	1:F:236:PHE:CE2	2.46	0.50
1:F:13:THR:OG1	1:F:87:THR:HA	2.12	0.49
1:C:114:LYS:NZ	1:F:106:ASP:OD1	2.45	0.49
1:C:196:THR:HG22	1:C:198:GLU:N	2.27	0.49
1:B:213:ILE:HG23	1:B:246:GLY:O	2.12	0.49
1:D:236:PHE:CD2	1:F:217:ALA:HB2	2.48	0.49
1:H:96:ALA:HA	1:H:147:ALA:HA	1.94	0.49
1:C:26:ASP:O	1:C:30:GLN:HG2	2.14	0.48
1:D:62:VAL:HB	1:D:115:ALA:HB1	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:34:VAL:HB	1:F:55:VAL:HG22	1.95	0.48
1:G:190:ALA:O	1:G:200:GLN:OE1	2.31	0.48
1:H:120:VAL:HG13	1:H:133:ILE:HD13	1.95	0.48
1:C:111:ARG:NH1	2:C:303:HOH:O	2.46	0.48
1:G:240:ALA:HA	1:H:250:GLN:NE2	2.27	0.48
1:G:76:ARG:HA	1:G:80:GLY:HA2	1.94	0.48
1:C:51:LEU:HB3	1:C:55:VAL:HG21	1.94	0.48
1:C:97:LEU:HG	1:F:124:LEU:HD11	1.95	0.48
1:D:56:ARG:HH21	1:D:79:GLU:CD	2.20	0.48
1:A:146:GLN:NE2	2:A:304:HOH:O	2.45	0.47
1:D:71:LEU:O	1:D:74:THR:HG22	2.14	0.47
1:E:98:GLY:N	1:H:121:GLN:OE1	2.41	0.47
1:F:94:MET:HB2	1:F:148:PHE:CE1	2.49	0.47
1:B:165:TRP:CD1	1:G:97:LEU:HD22	2.50	0.47
1:D:87:THR:O	1:D:136:ASN:HB2	2.14	0.47
1:C:71:LEU:O	1:C:74:THR:HG22	2.14	0.47
1:C:88:ASN:ND2	1:C:136:ASN:OD1	2.48	0.47
1:E:137:GLY:O	1:E:181:PRO:HD2	2.13	0.47
1:F:124:LEU:HB3	1:F:172:ARG:NH1	2.29	0.47
1:A:56:ARG:HH22	1:A:75:ILE:HG12	1.62	0.47
1:B:236:PHE:CD2	1:E:217:ALA:HB2	2.50	0.47
1:C:251:VAL:C	1:D:144:GLY:H	2.22	0.47
1:E:193:GLY:HA2	1:E:203:THR:HG21	1.96	0.47
1:G:44:LEU:O	1:G:48:VAL:HG12	2.14	0.47
1:C:118:PHE:O	1:C:122:LYS:HD3	2.15	0.47
1:E:39:ARG:CD	1:E:111:ARG:HH22	2.22	0.47
1:B:137:GLY:O	1:B:181:PRO:HD2	2.15	0.47
1:H:116:VAL:O	1:H:120:VAL:HG23	2.15	0.47
1:B:90:GLY:HA2	1:B:111:ARG:HG2	1.96	0.46
1:H:25:LYS:HA	1:H:53:GLN:HE22	1.80	0.46
1:B:155:LYS:HD2	1:B:155:LYS:HA	1.63	0.46
1:E:8:LYS:HD3	1:E:84:ILE:HD11	1.97	0.46
1:E:105:PHE:C	1:E:105:PHE:CD2	2.94	0.46
1:F:190:ALA:HB1	1:F:200:GLN:OE1	2.15	0.46
1:C:56:ARG:HH22	1:C:74:THR:HG23	1.81	0.46
1:C:59:ARG:O	1:C:59:ARG:HG2	2.14	0.46
1:E:35:ILE:HD13	1:E:75:ILE:HG12	1.96	0.46
1:G:155:LYS:HA	1:G:155:LYS:HD2	1.74	0.46
1:H:139:ILE:HG21	1:H:245:ASP:HB3	1.96	0.46
1:B:59:ARG:HG2	1:B:59:ARG:NH2	2.30	0.46
1:F:195:ASP:OD2	1:F:195:ASP:N	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:ALA:HB2	1:C:236:PHE:CD2	2.51	0.46
1:D:166:VAL:HG22	1:D:238:ASN:OD1	2.16	0.46
1:A:59:ARG:HH11	1:A:59:ARG:CG	1.99	0.46
1:D:94:MET:HE1	1:D:148:PHE:CE2	2.51	0.46
1:H:68:LEU:HB3	1:H:122:LYS:HD2	1.98	0.46
1:A:236:PHE:CE2	1:C:217:ALA:HB2	2.50	0.45
1:D:5:LEU:HD12	1:D:5:LEU:HA	1.77	0.45
1:A:35:ILE:HD13	1:A:75:ILE:HG12	1.98	0.45
1:D:235:SER:OG	1:F:221:GLU:OE2	2.26	0.45
1:E:61:ASP:OD1	1:E:111:ARG:NH1	2.38	0.45
1:F:127:MET:HE2	1:F:131:ALA:HB1	1.97	0.45
1:H:52:GLY:O	1:H:53:GLN:HG2	2.16	0.45
1:F:75:ILE:O	1:F:80:GLY:N	2.47	0.45
1:H:41:GLN:OE1	1:H:59:ARG:HD3	2.15	0.45
1:D:138:SER:HB3	1:D:155:LYS:HG3	1.98	0.45
1:A:35:ILE:HG12	1:A:56:ARG:HE	1.77	0.45
1:E:5:LEU:O	1:E:8:LYS:HB2	2.17	0.45
1:G:136:ASN:HB3	2:G:319:HOH:O	2.16	0.45
1:G:217:ALA:HB2	1:H:236:PHE:CD1	2.52	0.45
1:H:108:THR:O	1:H:112:ASN:HB2	2.17	0.45
1:H:213:ILE:HD12	1:H:215:ARG:HE	1.80	0.45
1:C:39:ARG:HG3	1:C:39:ARG:HH11	1.81	0.45
1:C:196:THR:O	1:C:200:GLN:HG3	2.16	0.45
1:G:245:ASP:OD1	1:G:245:ASP:N	2.49	0.45
1:G:217:ALA:HB2	1:H:236:PHE:CE1	2.51	0.44
1:H:131:ALA:HB3	1:H:174:ILE:HG12	1.99	0.44
1:E:39:ARG:HD2	1:E:61:ASP:CG	2.42	0.44
1:A:236:PHE:CD2	1:C:217:ALA:HB2	2.53	0.44
1:C:35:ILE:HG12	1:C:56:ARG:HE	1.83	0.44
1:D:155:LYS:HA	1:D:155:LYS:HD2	1.68	0.44
1:E:122:LYS:O	1:E:125:PRO:HD2	2.18	0.44
1:G:123:ALA:O	1:G:127:MET:HG3	2.18	0.44
1:C:159:ARG:HA	1:C:178:VAL:HG21	2.00	0.44
1:A:129:GLN:HG2	1:A:172:ARG:O	2.18	0.43
1:H:124:LEU:HD11	1:H:169:LEU:HD21	1.99	0.43
1:H:159:ARG:HA	1:H:178:VAL:HG21	2.00	0.43
1:A:124:LEU:HD11	1:D:97:LEU:HG	1.99	0.43
1:B:51:LEU:HD12	1:B:51:LEU:HA	1.81	0.43
1:E:34:VAL:HB	1:E:55:VAL:HG22	1.98	0.43
1:E:85:LEU:HD12	1:E:133:ILE:HG23	2.00	0.43
1:H:62:VAL:HB	1:H:115:ALA:HB1	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:ALA:HB2	1:C:236:PHE:CE2	2.54	0.43
1:B:35:ILE:HD13	1:B:75:ILE:HG12	2.00	0.43
1:D:186:THR:HG22	1:D:188:GLY:N	2.33	0.43
1:A:137:GLY:O	1:A:181:PRO:HD2	2.18	0.43
1:B:196:THR:O	1:B:200:GLN:HG3	2.19	0.43
1:A:138:SER:HB3	1:A:155:LYS:HG3	2.01	0.43
1:B:106:ASP:O	1:B:110:GLU:HB2	2.18	0.43
1:C:159:ARG:HD3	1:C:159:ARG:C	2.43	0.43
1:F:32:ALA:O	1:F:34:VAL:HG23	2.19	0.43
1:G:200:GLN:O	1:G:204:LEU:HD12	2.19	0.43
1:D:3:LYS:HE2	1:D:4:ARG:H	1.84	0.42
1:G:19:ILE:O	1:G:23:THR:OG1	2.29	0.42
1:D:42:ALA:O	1:D:46:GLN:HG3	2.20	0.42
1:D:224:LYS:HB3	1:F:233:ASP:HB3	2.00	0.42
1:H:181:PRO:HB3	1:H:222:ILE:HD12	2.02	0.42
1:A:96:ALA:HA	1:A:147:ALA:HA	2.01	0.42
1:B:128:PRO:HD2	1:B:131:ALA:HB2	2.01	0.42
1:F:134:ILE:N	1:F:134:ILE:HD12	2.35	0.42
1:G:6:GLU:H	1:G:6:GLU:HG3	1.48	0.42
1:F:15:GLY:HA3	1:F:36:ILE:HB	2.02	0.42
1:F:111:ARG:NH1	2:F:306:HOH:O	2.53	0.42
1:G:139:ILE:HG21	1:G:245:ASP:HB3	2.00	0.42
1:G:190:ALA:C	1:G:200:GLN:OE1	2.63	0.42
1:G:244:ALA:HB1	1:H:236:PHE:HB3	2.02	0.42
1:A:87:THR:O	1:A:136:ASN:HB2	2.20	0.42
1:F:84:ILE:HG12	1:F:230:ALA:HB1	2.02	0.42
1:G:242:ILE:HD13	1:H:242:ILE:HD13	2.01	0.42
1:H:94:MET:HE2	1:H:148:PHE:CE1	2.55	0.41
1:B:217:ALA:HB2	1:E:236:PHE:CE2	2.54	0.41
1:H:67:ASP:OD2	1:H:67:ASP:N	2.54	0.41
1:H:87:THR:O	1:H:136:ASN:HB2	2.20	0.41
1:A:196:THR:O	1:A:200:GLN:HG3	2.20	0.41
1:C:5:LEU:HD21	1:C:231:SER:HA	2.02	0.41
1:H:5:LEU:HD23	1:H:27:LEU:HD23	2.01	0.41
1:H:162:ALA:O	1:H:166:VAL:HG23	2.19	0.41
1:B:59:ARG:HG2	1:B:59:ARG:HH21	1.84	0.41
1:G:159:ARG:HA	1:G:178:VAL:HG21	2.03	0.41
1:H:51:LEU:HG	1:H:53:GLN:NE2	2.35	0.41
1:H:182:GLY:O	1:H:184:THR:HG23	2.20	0.41
1:H:71:LEU:O	1:H:75:ILE:HG13	2.21	0.41
1:H:124:LEU:HD23	1:H:124:LEU:HA	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:84:ILE:HG12	1:H:230:ALA:HB1	2.03	0.41
1:E:131:ALA:HB3	1:E:174:ILE:HD12	2.02	0.41
1:G:213:ILE:HD11	1:H:238:ASN:ND2	2.26	0.41
1:H:51:LEU:HD12	1:H:51:LEU:HA	1.87	0.41
1:D:3:LYS:HB2	1:D:4:ARG:H	1.69	0.41
1:D:169:LEU:HD12	1:D:176:VAL:HG22	2.03	0.41
1:E:120:VAL:HG21	1:E:165:TRP:CZ3	2.55	0.41
1:H:179:VAL:HG23	1:H:229:LEU:HD12	2.03	0.41
1:C:171:GLU:OE1	1:C:171:GLU:HA	2.20	0.40
1:B:187:ILE:HD13	1:B:187:ILE:HA	1.70	0.40
1:C:137:GLY:O	1:C:181:PRO:HD2	2.21	0.40
1:A:155:LYS:HA	1:A:155:LYS:HD2	1.84	0.40
1:D:236:PHE:CE1	1:F:213:ILE:HD11	2.55	0.40
1:C:114:LYS:HD3	1:F:105:PHE:CD2	2.56	0.40
1:E:140:LYS:HA	1:E:140:LYS:HD3	1.94	0.40
1:H:184:THR:CG2	1:H:217:ALA:HB3	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/251 (99%)	244 (98%)	4 (2%)	0	100	100
1	B	248/251 (99%)	246 (99%)	2 (1%)	0	100	100
1	C	247/251 (98%)	245 (99%)	2 (1%)	0	100	100
1	D	247/251 (98%)	245 (99%)	2 (1%)	0	100	100
1	E	247/251 (98%)	243 (98%)	4 (2%)	0	100	100
1	F	247/251 (98%)	244 (99%)	3 (1%)	0	100	100
1	G	246/251 (98%)	244 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	235/251 (94%)	232 (99%)	3 (1%)	0	100	100
All	All	1965/2008 (98%)	1943 (99%)	22 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	183/186 (98%)	173 (94%)	10 (6%)	19	31
1	B	182/186 (98%)	175 (96%)	7 (4%)	29	46
1	C	180/186 (97%)	169 (94%)	11 (6%)	17	27
1	D	182/186 (98%)	173 (95%)	9 (5%)	22	36
1	E	181/186 (97%)	171 (94%)	10 (6%)	19	31
1	F	177/186 (95%)	167 (94%)	10 (6%)	19	30
1	G	174/186 (94%)	156 (90%)	18 (10%)	7	9
1	H	164/186 (88%)	149 (91%)	15 (9%)	9	13
All	All	1423/1488 (96%)	1333 (94%)	90 (6%)	16	26

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	51	LEU
1	A	56	ARG
1	A	59	ARG
1	A	60	SER
1	A	176	VAL
1	A	185	ARG
1	A	187	ILE
1	A	189	LEU
1	A	196	THR

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Mol	Chain	Res	Type
1	B	4	ARG
1	B	51	LEU
1	B	60	SER
1	B	176	VAL
1	B	187	ILE
1	B	195	ASP
1	B	196	THR
1	C	3	LYS
1	C	59	ARG
1	C	60	SER
1	C	65	SER
1	C	73	GLU
1	C	100	ILE
1	C	110	GLU
1	C	176	VAL
1	C	183	SER
1	C	195	ASP
1	C	197	GLN
1	D	3	LYS
1	D	5	LEU
1	D	6	GLU
1	D	37	THR
1	D	39	ARG
1	D	155	LYS
1	D	176	VAL
1	D	183	SER
1	D	210	LEU
1	E	3	LYS
1	E	56	ARG
1	E	85	LEU
1	E	93	SER
1	E	99	GLU
1	E	101	SER
1	E	124	LEU
1	E	176	VAL
1	E	196	THR
1	E	216	LEU
1	F	4	ARG
1	F	60	SER
1	F	74	THR
1	F	93	SER
1	F	146	GLN

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Mol	Chain	Res	Type
1	F	176	VAL
1	F	186	THR
1	F	195	ASP
1	F	196	THR
1	F	198	GLU
1	G	4	ARG
1	G	6	GLU
1	G	30	GLN
1	G	51	LEU
1	G	53	GLN
1	G	74	THR
1	G	122	LYS
1	G	124	LEU
1	G	166	VAL
1	G	170	LYS
1	G	171	GLU
1	G	176	VAL
1	G	183	SER
1	G	186	THR
1	G	195	ASP
1	G	197	GLN
1	G	200	GLN
1	G	231	SER
1	H	6	GLU
1	H	13	THR
1	H	35	ILE
1	H	44	LEU
1	H	55	VAL
1	H	71	LEU
1	H	73	GLU
1	H	87	THR
1	H	102	GLU
1	H	134	ILE
1	H	163	ARG
1	H	176	VAL
1	H	192	LEU
1	H	204	LEU
1	H	235	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	53	GLN
1	A	129	GLN
1	A	136	ASN
1	A	146	GLN
1	A	197	GLN
1	B	30	GLN
1	B	103	GLN
1	C	88	ASN
1	C	136	ASN
1	C	250	GLN
1	D	88	ASN
1	D	200	GLN
1	E	103	GLN
1	F	41	GLN
1	F	250	GLN
1	G	104	HIS
1	G	250	GLN
1	H	88	ASN
1	H	146	GLN
1	H	177	ASN
1	H	250	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 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	250/251 (99%)	0.37	23 (9%) 14 13	27, 37, 72, 121	0
1	B	250/251 (99%)	0.46	22 (8%) 15 14	31, 41, 74, 114	0
1	C	249/251 (99%)	0.93	42 (16%) 4 4	31, 48, 79, 112	0
1	D	249/251 (99%)	0.95	39 (15%) 5 4	31, 50, 81, 110	0
1	E	249/251 (99%)	1.16	41 (16%) 4 4	36, 54, 81, 118	0
1	F	249/251 (99%)	1.30	48 (19%) 3 3	33, 50, 83, 125	0
1	G	248/251 (98%)	1.60	78 (31%) 1 1	34, 59, 93, 131	0
1	H	239/251 (95%)	2.92	165 (69%) 0 0	42, 70, 110, 154	0
All	All	1983/2008 (98%)	1.20	458 (23%) 2 1	27, 50, 90, 154	0

All (458) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	195	ASP	8.3
1	H	14	GLY	7.6
1	H	187	ILE	7.6
1	H	49	ALA	7.5
1	H	48	VAL	7.4
1	H	5	LEU	7.1
1	H	55	VAL	7.1
1	H	204	LEU	6.9
1	H	202	GLY	6.7
1	H	52	GLY	6.7
1	C	196	THR	6.6
1	A	196	THR	6.6
1	E	196	THR	6.5
1	H	186	THR	6.4
1	H	190	ALA	6.4
1	H	53	GLN	6.3

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Mol	Chain	Res	Type	RSRZ
1	H	17	SER	6.3
1	H	39	ARG	6.1
1	C	53	GLN	6.1
1	H	40	ARG	6.0
1	G	196	THR	5.9
1	C	3	LYS	5.9
1	H	193	GLY	5.9
1	H	21	LEU	5.9
1	H	26	ASP	5.8
1	H	51	LEU	5.8
1	D	3	LYS	5.6
1	H	32	ALA	5.5
1	H	80	GLY	5.5
1	H	44	LEU	5.5
1	H	192	LEU	5.5
1	D	53	GLN	5.4
1	B	198	GLU	5.3
1	H	185	ARG	5.3
1	G	4	ARG	5.2
1	F	3	LYS	5.1
1	G	233	ASP	5.1
1	H	19	ILE	5.0
1	D	4	ARG	5.0
1	B	197	GLN	5.0
1	A	2	SER	5.0
1	H	86	PHE	5.0
1	H	16	THR	5.0
1	H	225	VAL	4.9
1	E	187	ILE	4.9
1	H	218	ASP	4.9
1	B	194	GLY	4.9
1	F	52	GLY	4.9
1	D	193	GLY	4.9
1	G	6	GLU	4.8
1	C	195	ASP	4.7
1	E	53	GLN	4.7
1	H	203	THR	4.7
1	F	194	GLY	4.7
1	H	77	ALA	4.7
1	H	46	GLN	4.7
1	G	198	GLU	4.7
1	H	57	GLY	4.7

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Mol	Chain	Res	Type	RSRZ
1	F	192	LEU	4.6
1	G	5	LEU	4.6
1	E	39	ARG	4.6
1	H	41	GLN	4.6
1	H	27	LEU	4.6
1	B	2	SER	4.6
1	H	37	THR	4.6
1	D	194	GLY	4.5
1	H	79	GLU	4.5
1	H	110	GLU	4.5
1	F	81	ARG	4.5
1	C	194	GLY	4.5
1	B	195	ASP	4.5
1	H	42	ALA	4.5
1	G	53	GLN	4.5
1	H	78	THR	4.4
1	H	43	GLU	4.4
1	H	18	GLY	4.4
1	F	187	ILE	4.4
1	H	36	ILE	4.4
1	H	65	SER	4.4
1	F	80	GLY	4.3
1	F	196	THR	4.3
1	D	199	GLY	4.3
1	E	111	ARG	4.3
1	G	9	VAL	4.2
1	A	56	ARG	4.2
1	H	89	ALA	4.2
1	H	88	ASN	4.2
1	H	30	GLN	4.2
1	H	31	GLY	4.2
1	A	197	GLN	4.2
1	F	30	GLN	4.2
1	G	175	ARG	4.2
1	B	196	THR	4.2
1	H	15	GLY	4.1
1	C	52	GLY	4.1
1	H	60	SER	4.1
1	H	205	ALA	4.1
1	H	13	THR	4.1
1	H	54	GLY	4.1
1	C	76	ARG	4.0

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Mol	Chain	Res	Type	RSRZ
1	F	198	GLU	4.0
1	B	3	LYS	4.0
1	H	181	PRO	4.0
1	H	82	LEU	4.0
1	F	4	ARG	4.0
1	D	187	ILE	3.9
1	G	172	ARG	3.9
1	B	53	GLN	3.9
1	G	197	GLN	3.9
1	H	103	GLN	3.9
1	A	193	GLY	3.9
1	H	20	GLY	3.9
1	C	4	ARG	3.9
1	E	4	ARG	3.9
1	E	6	GLU	3.9
1	H	50	ALA	3.9
1	H	131	ALA	3.9
1	H	230	ALA	3.9
1	C	5	LEU	3.9
1	G	8	LYS	3.9
1	A	199	GLY	3.9
1	H	33	ARG	3.9
1	G	171	GLU	3.8
1	H	188	GLY	3.8
1	G	51	LEU	3.8
1	G	76	ARG	3.8
1	H	75	ILE	3.8
1	B	185	ARG	3.8
1	C	78	THR	3.7
1	H	87	THR	3.7
1	G	56	ARG	3.7
1	H	76	ARG	3.7
1	D	197	GLN	3.7
1	H	9	VAL	3.7
1	C	89	ALA	3.7
1	G	173	GLY	3.6
1	D	196	THR	3.6
1	G	17	SER	3.6
1	G	7	GLY	3.6
1	H	56	ARG	3.6
1	H	62	VAL	3.6
1	G	33	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
1	G	81	ARG	3.6
1	H	189	LEU	3.6
1	H	112	ASN	3.6
1	F	53	GLN	3.6
1	H	64	ARG	3.6
1	H	111	ARG	3.6
1	F	31	GLY	3.6
1	F	199	GLY	3.6
1	A	198	GLU	3.6
1	D	198	GLU	3.6
1	H	22	ALA	3.6
1	E	40	ARG	3.5
1	A	194	GLY	3.5
1	F	62	VAL	3.5
1	E	64	ARG	3.5
1	G	29	ALA	3.5
1	D	94	MET	3.5
1	G	54	GLY	3.5
1	H	71	LEU	3.5
1	H	221	GLU	3.5
1	F	190	ALA	3.5
1	C	51	LEU	3.5
1	G	124	LEU	3.5
1	H	7	GLY	3.4
1	H	120	VAL	3.4
1	A	192	LEU	3.4
1	E	195	ASP	3.4
1	G	30	GLN	3.4
1	E	62	VAL	3.4
1	F	59	ARG	3.4
1	H	90	GLY	3.4
1	F	197	GLN	3.4
1	H	124	LEU	3.4
1	H	10	ALA	3.4
1	A	195	ASP	3.4
1	H	8	LYS	3.3
1	E	7	GLY	3.3
1	B	4	ARG	3.3
1	C	54	GLY	3.3
1	G	52	GLY	3.3
1	G	89	ALA	3.2
1	H	24	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	H	223	ALA	3.2
1	G	194	GLY	3.2
1	F	195	ASP	3.2
1	G	195	ASP	3.2
1	H	68	LEU	3.2
1	H	138	SER	3.2
1	G	32	ALA	3.2
1	D	188	GLY	3.2
1	H	23	THR	3.2
1	D	148	PHE	3.2
1	H	235	SER	3.2
1	H	206	TYR	3.2
1	H	182	GLY	3.2
1	A	190	ALA	3.2
1	D	62	VAL	3.2
1	C	41	GLN	3.2
1	C	58	VAL	3.1
1	B	52	GLY	3.1
1	H	173	GLY	3.1
1	H	29	ALA	3.1
1	A	185	ARG	3.1
1	H	175	ARG	3.1
1	H	35	ILE	3.1
1	H	94	MET	3.1
1	H	222	ILE	3.1
1	H	99	GLU	3.1
1	H	96	ALA	3.1
1	H	117	VAL	3.1
1	F	191	GLU	3.0
1	H	38	GLY	3.0
1	H	67	ASP	3.0
1	H	72	PHE	3.0
1	D	192	LEU	3.0
1	H	174	ILE	3.0
1	H	220	SER	3.0
1	C	110	GLU	3.0
1	H	12	VAL	3.0
1	G	38	GLY	3.0
1	C	73	GLU	3.0
1	E	89	ALA	3.0
1	E	99	GLU	3.0
1	G	49	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	5	LEU	3.0
1	C	40	ARG	3.0
1	G	25	LYS	3.0
1	G	31	GLY	3.0
1	H	191	GLU	3.0
1	A	189	LEU	2.9
1	G	187	ILE	2.9
1	H	184	THR	2.9
1	C	43	GLU	2.9
1	G	50	ALA	2.9
1	D	33	ARG	2.9
1	G	184	THR	2.9
1	H	180	SER	2.9
1	B	192	LEU	2.9
1	H	66	ALA	2.9
1	H	109	PHE	2.9
1	D	54	GLY	2.9
1	E	98	GLY	2.9
1	H	219	PRO	2.9
1	D	64	ARG	2.9
1	D	185	ARG	2.9
1	D	51	LEU	2.9
1	G	10	ALA	2.9
1	H	126	LEU	2.9
1	H	34	VAL	2.9
1	D	191	GLU	2.9
1	G	186	THR	2.9
1	G	213	ILE	2.9
1	G	170	LYS	2.8
1	G	46	GLN	2.8
1	B	187	ILE	2.8
1	H	69	ASP	2.8
1	G	193	GLY	2.8
1	F	82	LEU	2.8
1	E	118	PHE	2.8
1	G	48	VAL	2.8
1	A	4	ARG	2.8
1	C	81	ARG	2.8
1	F	64	ARG	2.8
1	F	74	THR	2.8
1	F	193	GLY	2.8
1	C	30	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	H	73	GLU	2.8
1	H	95	ALA	2.8
1	C	187	ILE	2.8
1	C	45	ASP	2.8
1	G	217	ALA	2.8
1	H	45	ASP	2.7
1	A	188	GLY	2.7
1	H	231	SER	2.7
1	C	191	GLU	2.7
1	F	56	ARG	2.7
1	H	28	ALA	2.7
1	H	81	ARG	2.7
1	G	218	ASP	2.7
1	G	237	ILE	2.7
1	H	136	ASN	2.7
1	E	38	GLY	2.7
1	F	54	GLY	2.7
1	D	99	GLU	2.7
1	F	29	ALA	2.7
1	C	6	GLU	2.7
1	C	59	ARG	2.7
1	H	58	VAL	2.7
1	F	19	ILE	2.7
1	G	183	SER	2.7
1	A	59	ARG	2.7
1	H	207	LEU	2.7
1	A	89	ALA	2.6
1	E	129	GLN	2.6
1	G	28	ALA	2.6
1	H	244	ALA	2.6
1	G	148	PHE	2.6
1	D	171	GLU	2.6
1	H	226	VAL	2.6
1	D	7	GLY	2.6
1	E	192	LEU	2.6
1	E	188	GLY	2.6
1	F	200	GLN	2.6
1	E	8	LYS	2.6
1	G	191	GLU	2.6
1	E	136	ASN	2.6
1	G	228	PHE	2.6
1	B	93	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	197	GLN	2.6
1	A	204	LEU	2.6
1	F	171	GLU	2.6
1	H	6	GLU	2.6
1	F	28	ALA	2.6
1	H	208	ALA	2.6
1	H	217	ALA	2.6
1	F	16	THR	2.6
1	G	202	GLY	2.6
1	G	200	GLN	2.5
1	H	216	LEU	2.5
1	D	190	ALA	2.5
1	G	123	ALA	2.5
1	H	92	ALA	2.5
1	H	147	ALA	2.5
1	D	52	GLY	2.5
1	F	148	PHE	2.5
1	H	59	ARG	2.5
1	C	124	LEU	2.5
1	F	94	MET	2.5
1	F	32	ALA	2.5
1	E	165	TRP	2.5
1	A	187	ILE	2.5
1	F	79	GLU	2.5
1	D	189	LEU	2.5
1	F	7	GLY	2.5
1	F	188	GLY	2.5
1	G	199	GLY	2.5
1	H	74	THR	2.5
1	G	19	ILE	2.5
1	H	251	VAL	2.5
1	H	11	LEU	2.5
1	B	54	GLY	2.5
1	C	199	GLY	2.5
1	H	183	SER	2.4
1	G	55	VAL	2.4
1	F	21	LEU	2.4
1	H	83	ASP	2.4
1	H	233	ASP	2.4
1	C	197	GLN	2.4
1	D	40	ARG	2.4
1	E	93	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	25	LYS	2.4
1	E	94	MET	2.4
1	G	192	LEU	2.4
1	H	61	ASP	2.4
1	G	20	GLY	2.4
1	H	130	GLY	2.4
1	H	135	LEU	2.4
1	F	172	ARG	2.4
1	H	249	ALA	2.4
1	G	243	THR	2.4
1	H	224	LYS	2.4
1	H	93	SER	2.4
1	G	94	MET	2.4
1	G	40	ARG	2.4
1	B	191	GLU	2.4
1	E	66	ALA	2.3
1	G	190	ALA	2.3
1	C	55	VAL	2.3
1	F	55	VAL	2.3
1	H	236	PHE	2.3
1	H	215	ARG	2.3
1	G	11	LEU	2.3
1	H	97	LEU	2.3
1	A	171	GLU	2.3
1	G	214	GLY	2.3
1	H	100	ILE	2.3
1	H	104	HIS	2.3
1	G	21	LEU	2.3
1	G	229	LEU	2.3
1	E	33	ARG	2.3
1	E	76	ARG	2.3
1	C	198	GLU	2.3
1	H	113	VAL	2.3
1	E	3	LYS	2.3
1	F	83	ASP	2.3
1	E	194	GLY	2.3
1	G	57	GLY	2.3
1	H	91	GLY	2.3
1	C	94	MET	2.3
1	E	172	ARG	2.3
1	E	52	GLY	2.2
1	G	185	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	49	ALA	2.2
1	C	108	THR	2.2
1	B	204	LEU	2.2
1	G	84	ILE	2.2
1	D	55	VAL	2.2
1	H	176	VAL	2.2
1	C	72	PHE	2.2
1	H	148	PHE	2.2
1	G	83	ASP	2.2
1	B	214	GLY	2.2
1	D	49	ALA	2.2
1	H	47	ALA	2.2
1	H	70	ALA	2.2
1	F	17	SER	2.2
1	G	204	LEU	2.2
1	H	102	GLU	2.2
1	A	202	GLY	2.2
1	B	200	GLN	2.2
1	E	167	LEU	2.1
1	F	75	ILE	2.1
1	G	75	ILE	2.1
1	A	3	LYS	2.1
1	H	125	PRO	2.1
1	E	193	GLY	2.1
1	D	63	THR	2.1
1	E	63	THR	2.1
1	G	77	ALA	2.1
1	H	153	ALA	2.1
1	H	172	ARG	2.1
1	B	94	MET	2.1
1	G	189	LEU	2.1
1	H	139	ILE	2.1
1	C	79	GLU	2.1
1	H	118	PHE	2.1
1	C	193	GLY	2.1
1	B	186	THR	2.1
1	C	56	ARG	2.1
1	C	42	ALA	2.1
1	E	100	ILE	2.1
1	F	134	ILE	2.1
1	D	48	VAL	2.1
1	D	128	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	246	GLY	2.1
1	F	175	ARG	2.1
1	C	8	LYS	2.1
1	E	68	LEU	2.1
1	A	201	ASP	2.1
1	B	201	ASP	2.1
1	D	90	GLY	2.1
1	D	39	ARG	2.1
1	D	78	THR	2.0
1	G	235	SER	2.0
1	E	5	LEU	2.0
1	F	51	LEU	2.0
1	E	198	GLU	2.0
1	H	127	MET	2.0
1	H	63	THR	2.0
1	H	171	GLU	2.0
1	D	89	ALA	2.0
1	F	146	GLN	2.0
1	C	192	LEU	2.0
1	E	201	ASP	2.0
1	G	27	LEU	2.0
1	C	111	ARG	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.