



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:09 PM UTC

PDB ID : 6AKF / pdb_00006akf
Title : Crystal structure of mouse claudin-3 P134A mutant in complex with C-terminal fragment of Clostridium perfringens enterotoxin
Authors : Nakamura, S.; Irie, K.; Fujiyoshi, Y.
Deposited on : 2018-08-31
Resolution : 3.90 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:

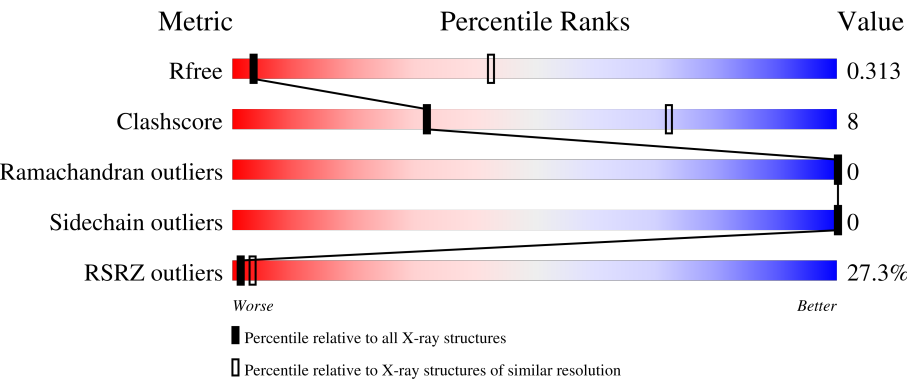
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.90 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.



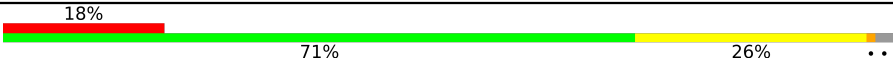
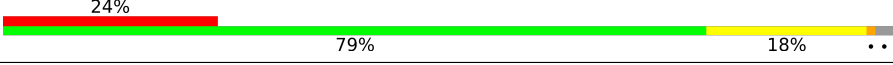
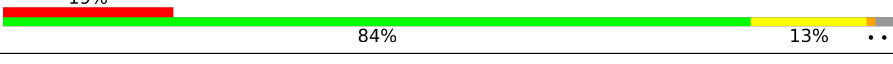
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1270 (4.10-3.70)
Clashscore	190562	1034 (4.08-3.72)
Ramachandran outliers	187476	1251 (4.10-3.70)
Sidechain outliers	187428	1243 (4.10-3.70)
RSRZ outliers	180081	1269 (4.10-3.70)

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	190	29% 78%18%..
1	C	190	25% 77%21%.
1	E	190	38% 78%13%.8%
1	G	190	31% 76%13%11%
2	B	119	13% 76%21%..

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Mol	Chain	Length	Quality of chain
2	D	119	
2	F	119	
2	H	119	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8888 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 Claudin-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	184	Total	C	N	O	S	0	0	0
			1335	869	217	237	12			
1	C	186	Total	C	N	O	S	0	0	0
			1350	876	220	242	12			
1	E	174	Total	C	N	O	S	0	0	0
			1264	825	206	221	12			
1	G	169	Total	C	N	O	S	0	0	0
			1222	800	198	213	11			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	see sequence details	UNP Q9Z0G9
A	-5	HIS	-	see sequence details	UNP Q9Z0G9
A	-4	MET	-	see sequence details	UNP Q9Z0G9
A	-3	ALA	-	see sequence details	UNP Q9Z0G9
A	-2	SER	-	see sequence details	UNP Q9Z0G9
A	-1	GLY	-	see sequence details	UNP Q9Z0G9
A	0	SER	-	see sequence details	UNP Q9Z0G9
A	103	ALA	CYS	engineered mutation	UNP Q9Z0G9
A	106	ALA	CYS	engineered mutation	UNP Q9Z0G9
A	134	ALA	PRO	engineered mutation	UNP Q9Z0G9
A	181	ALA	CYS	engineered mutation	UNP Q9Z0G9
A	182	ALA	CYS	engineered mutation	UNP Q9Z0G9
C	-6	GLY	-	see sequence details	UNP Q9Z0G9
C	-5	HIS	-	see sequence details	UNP Q9Z0G9
C	-4	MET	-	see sequence details	UNP Q9Z0G9
C	-3	ALA	-	see sequence details	UNP Q9Z0G9
C	-2	SER	-	see sequence details	UNP Q9Z0G9
C	-1	GLY	-	see sequence details	UNP Q9Z0G9
C	0	SER	-	see sequence details	UNP Q9Z0G9
C	103	ALA	CYS	engineered mutation	UNP Q9Z0G9
C	106	ALA	CYS	engineered mutation	UNP Q9Z0G9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	134	ALA	PRO	engineered mutation	UNP Q9Z0G9
C	181	ALA	CYS	engineered mutation	UNP Q9Z0G9
C	182	ALA	CYS	engineered mutation	UNP Q9Z0G9
E	-6	GLY	-	see sequence details	UNP Q9Z0G9
E	-5	HIS	-	see sequence details	UNP Q9Z0G9
E	-4	MET	-	see sequence details	UNP Q9Z0G9
E	-3	ALA	-	see sequence details	UNP Q9Z0G9
E	-2	SER	-	see sequence details	UNP Q9Z0G9
E	-1	GLY	-	see sequence details	UNP Q9Z0G9
E	0	SER	-	see sequence details	UNP Q9Z0G9
E	103	ALA	CYS	engineered mutation	UNP Q9Z0G9
E	106	ALA	CYS	engineered mutation	UNP Q9Z0G9
E	134	ALA	PRO	engineered mutation	UNP Q9Z0G9
E	181	ALA	CYS	engineered mutation	UNP Q9Z0G9
E	182	ALA	CYS	engineered mutation	UNP Q9Z0G9
G	-6	GLY	-	see sequence details	UNP Q9Z0G9
G	-5	HIS	-	see sequence details	UNP Q9Z0G9
G	-4	MET	-	see sequence details	UNP Q9Z0G9
G	-3	ALA	-	see sequence details	UNP Q9Z0G9
G	-2	SER	-	see sequence details	UNP Q9Z0G9
G	-1	GLY	-	see sequence details	UNP Q9Z0G9
G	0	SER	-	see sequence details	UNP Q9Z0G9
G	103	ALA	CYS	engineered mutation	UNP Q9Z0G9
G	106	ALA	CYS	engineered mutation	UNP Q9Z0G9
G	134	ALA	PRO	engineered mutation	UNP Q9Z0G9
G	181	ALA	CYS	engineered mutation	UNP Q9Z0G9
G	182	ALA	CYS	engineered mutation	UNP Q9Z0G9

- Molecule 2 is a protein called Heat-labile enterotoxin B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	117	Total	C	N	O	S	0	0	0
			925	591	155	178	1			
2	D	117	Total	C	N	O	S	0	0	0
			932	595	157	179	1			
2	F	117	Total	C	N	O	S	0	0	0
			928	592	156	179	1			
2	H	117	Total	C	N	O	S	0	0	0
			932	595	157	179	1			

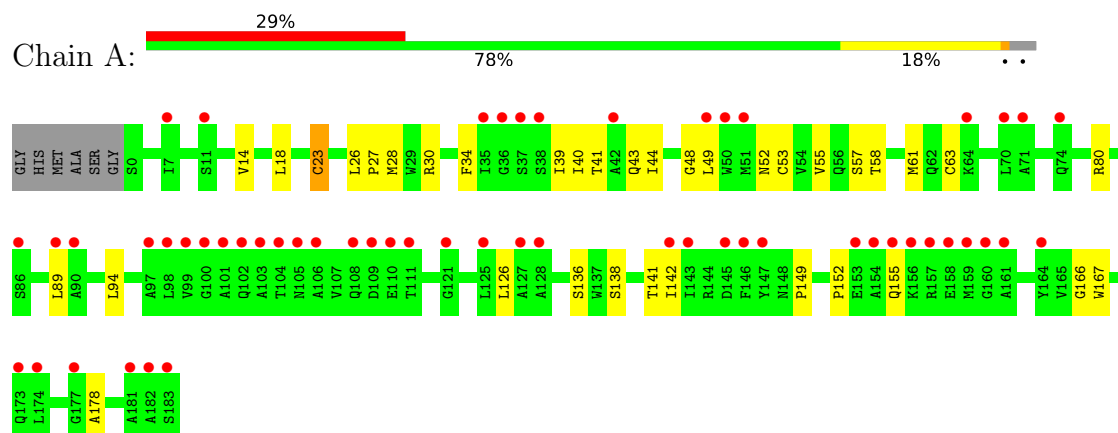
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	201	GLY	-	see sequence details	UNP P01558
B	202	SER	-	see sequence details	UNP P01558
B	313	ALA	SER	engineered mutation	UNP P01558
D	201	GLY	-	see sequence details	UNP P01558
D	202	SER	-	see sequence details	UNP P01558
D	313	ALA	SER	engineered mutation	UNP P01558
F	201	GLY	-	see sequence details	UNP P01558
F	202	SER	-	see sequence details	UNP P01558
F	313	ALA	SER	engineered mutation	UNP P01558
H	201	GLY	-	see sequence details	UNP P01558
H	202	SER	-	see sequence details	UNP P01558
H	313	ALA	SER	engineered mutation	UNP P01558

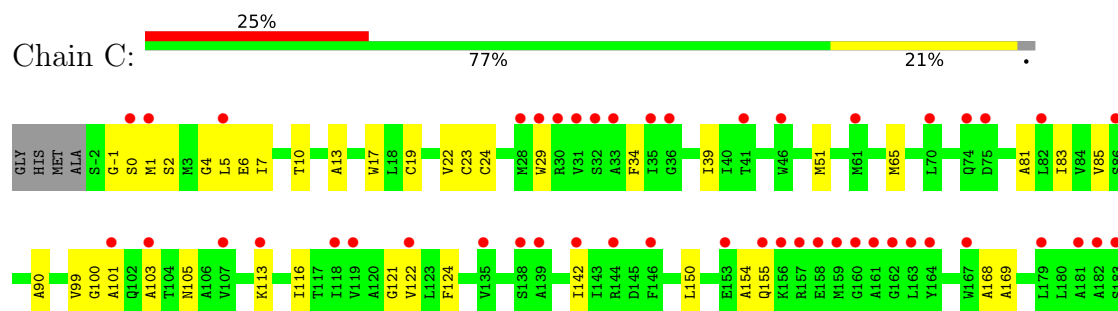
3 Residue-property plots [i](#)

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.

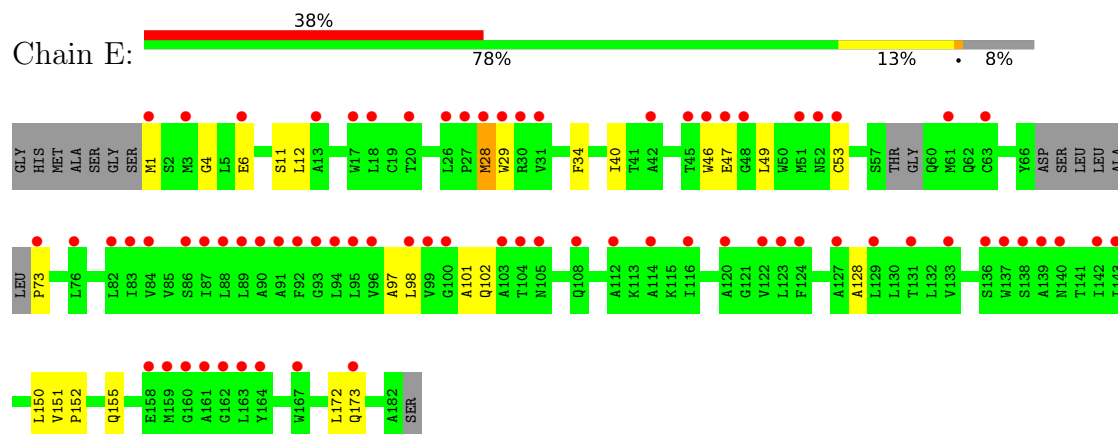
• Molecule 1: Claudin-3



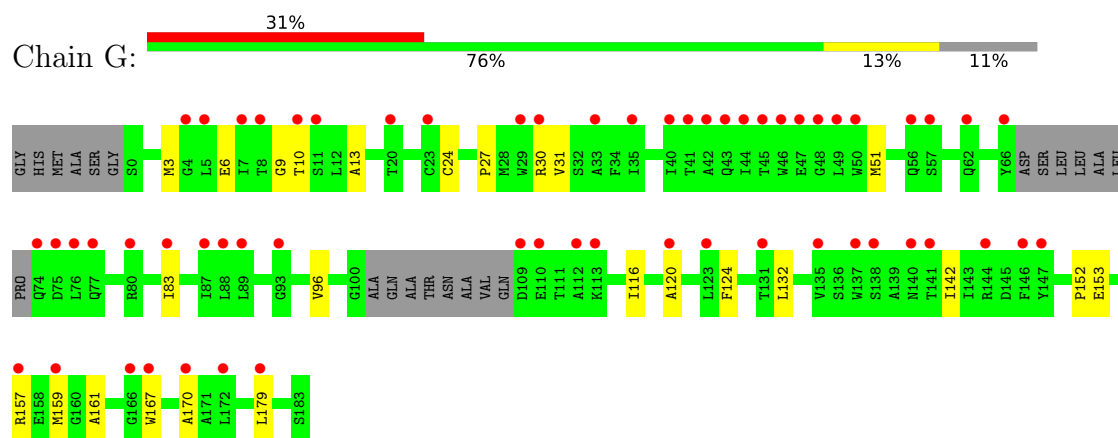
• Molecule 1: Claudin-3



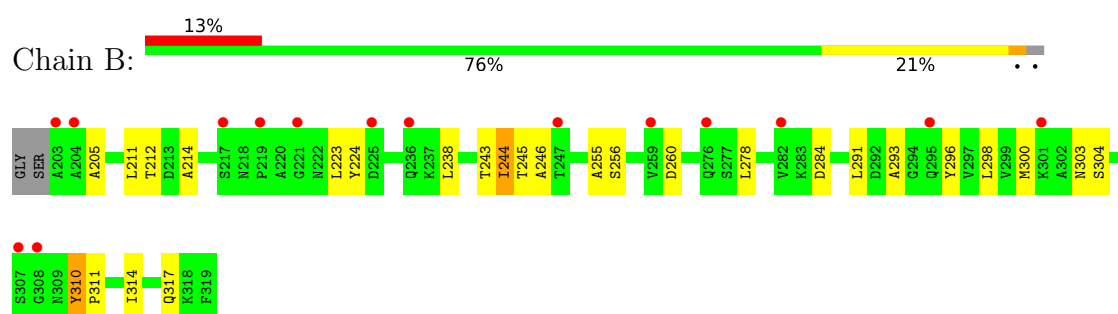
• Molecule 1: Claudin-3



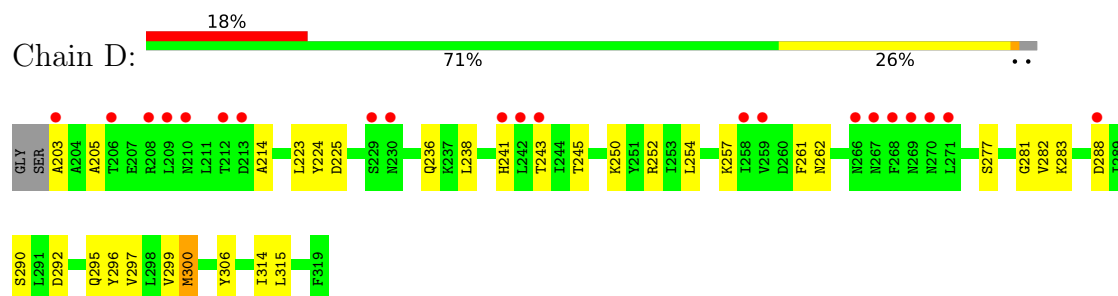
● Molecule 1: Claudin-3



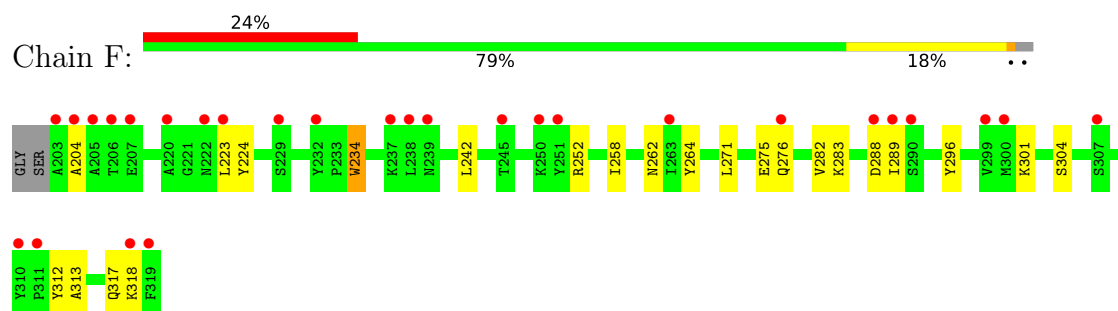
● Molecule 2: Heat-labile enterotoxin B chain



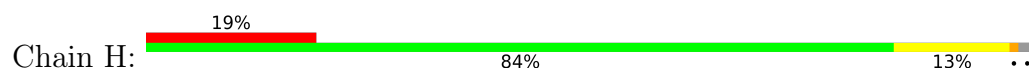
● Molecule 2: Heat-labile enterotoxin B chain

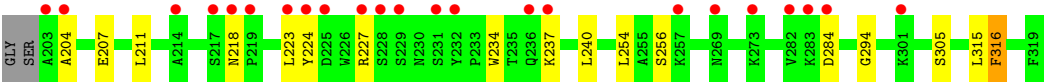


● Molecule 2: Heat-labile enterotoxin B chain



● Molecule 2: Heat-labile enterotoxin B chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	69.54Å 127.45Å 165.70Å 90.00° 104.53° 90.00°	Depositor
Resolution (Å)	46.66 – 3.90 46.66 – 3.90	Depositor EDS
% Data completeness (in resolution range)	98.6 (46.66-3.90) 98.6 (46.66-3.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 3.88Å)	Xtriage
Refinement program	PHENIX 1.13_2998, REFMAC 5	Depositor
R, R_{free}	0.274 , 0.312 0.273 , 0.313	Depositor DCC
R_{free} test set	1314 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	95.6	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 34.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.065 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	8888	wwPDB-VP
Average B, all atoms (Å ²)	119.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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	0.80	0/1357	1.12	6/1855 (0.3%)
1	C	0.75	0/1372	1.14	4/1875 (0.2%)
1	E	0.83	0/1284	1.11	5/1753 (0.3%)
1	G	0.87	1/1241 (0.1%)	1.07	3/1694 (0.2%)
2	B	0.76	0/946	1.08	4/1288 (0.3%)
2	D	0.70	0/953	0.98	2/1296 (0.2%)
2	F	0.79	0/949	0.96	4/1292 (0.3%)
2	H	0.71	0/953	1.01	3/1296 (0.2%)
All	All	0.78	1/9055 (0.0%)	1.07	31/12349 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	27	PRO	N-CD	-13.45	1.28	1.47

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	7	ILE	N-CA-C	13.67	123.55	110.42
2	D	282	VAL	N-CA-C	8.70	119.54	111.45
1	A	40	ILE	N-CA-C	7.72	119.01	111.67
1	G	27	PRO	N-CA-CB	-7.72	97.64	102.81
1	E	98	LEU	N-CA-C	7.67	123.30	111.56
1	A	40	ILE	CB-CA-C	-7.50	102.95	111.80
2	B	245	THR	N-CA-C	7.39	122.42	113.41
1	C	0	SER	N-CA-C	7.11	122.33	112.45
1	C	-1	GLY	N-CA-C	6.71	129.08	113.18
1	A	26	LEU	N-CA-C	6.37	117.73	109.64
1	C	1	MET	N-CA-C	-6.35	105.36	113.23
2	H	211	LEU	N-CA-C	6.26	118.63	111.11
1	G	27	PRO	CA-N-CD	6.06	120.48	112.00
2	F	224	TYR	N-CA-C	5.98	119.24	108.48
1	E	47	GLU	N-CA-C	5.95	117.73	110.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	318	LYS	N-CA-C	5.86	119.25	107.41
2	D	300	MET	N-CA-C	5.84	117.89	108.32
2	H	316	PHE	CB-CA-C	-5.77	100.58	110.22
2	H	294	GLY	N-CA-C	5.73	117.62	110.29
2	B	310	TYR	CB-CA-C	-5.64	102.78	110.22
1	A	178	ALA	N-CA-C	5.61	117.25	111.03
2	B	244	ILE	N-CA-C	5.58	116.16	108.12
2	B	256	SER	N-CA-C	5.52	117.65	110.53
2	F	234	TRP	N-CA-C	5.48	117.26	111.28
1	A	23	CYS	N-CA-C	5.33	116.77	111.07
2	F	204	ALA	N-CA-C	5.25	116.83	108.79
1	A	41	THR	N-CA-C	-5.24	98.85	108.02
1	E	28	MET	N-CA-C	-5.16	96.88	107.67
1	E	53	CYS	N-CA-C	5.13	117.63	107.98
1	E	29	TRP	N-CA-C	-5.09	107.13	113.55
1	G	161	ALA	N-CA-C	5.04	118.91	112.87

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	1335	0	1387	23	0
1	C	1350	0	1404	25	0
1	E	1264	0	1306	28	0
1	G	1222	0	1262	18	0
2	B	925	0	892	26	0
2	D	932	0	907	19	0
2	F	928	0	896	16	0
2	H	932	0	907	10	0
All	All	8888	0	8961	142	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 8.

All (142) 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)
2:B:211:LEU:HB3	2:B:244:ILE:HD11	1.21	1.14
2:B:205:ALA:HB3	2:B:238:LEU:HA	1.30	1.09
2:B:211:LEU:HB3	2:B:244:ILE:CD1	1.91	0.98
1:E:97:ALA:O	1:E:101:ALA:HB2	1.74	0.88
1:E:97:ALA:O	1:E:101:ALA:CB	2.30	0.79
2:B:211:LEU:CB	2:B:244:ILE:HD11	2.11	0.77
1:A:18:LEU:HD12	1:C:168:ALA:HB1	1.67	0.75
2:D:257:LYS:HD2	2:D:281:GLY:O	1.86	0.74
1:A:34:PHE:CE2	2:B:223:LEU:HD21	2.24	0.73
1:E:49:LEU:HD21	1:E:73:PRO:HB2	1.70	0.72
1:E:102:GLN:NE2	1:G:31:VAL:HG21	2.07	0.69
2:F:234:TRP:O	2:F:301:LYS:NZ	2.22	0.69
1:A:52:ASN:OD1	1:A:53:CYS:N	2.27	0.67
1:E:49:LEU:HD23	1:E:73:PRO:HG2	1.76	0.67
2:B:212:THR:HG23	2:B:244:ILE:HG23	1.76	0.66
1:E:34:PHE:HE2	2:F:223:LEU:HD21	1.60	0.65
1:C:155:GLN:HE21	2:D:225:ASP:HA	1.60	0.65
2:D:245:THR:O	2:D:245:THR:HG23	1.97	0.65
1:G:51:MET:SD	1:G:51:MET:N	2.70	0.64
1:C:34:PHE:CD2	2:D:223:LEU:HD21	2.32	0.64
2:B:205:ALA:HB1	2:B:238:LEU:HD13	1.80	0.63
2:B:243:THR:O	2:B:244:ILE:HD13	1.98	0.62
2:F:242:LEU:HB2	2:F:296:TYR:HB2	1.81	0.61
1:E:102:GLN:HE22	1:G:31:VAL:HG11	1.66	0.61
1:E:34:PHE:CE2	2:F:223:LEU:HD21	2.36	0.61
2:D:205:ALA:HB3	2:D:238:LEU:HA	1.83	0.61
1:A:27:PRO:HA	1:A:48:GLY:HA3	1.83	0.60
2:B:260:ASP:HB3	2:B:278:LEU:HD23	1.82	0.59
2:H:204:ALA:HB1	2:H:237:LYS:O	2.02	0.59
2:D:214:ALA:HB1	2:D:224:TYR:CE1	2.39	0.57
2:F:282:VAL:HG12	2:F:283:LYS:HG3	1.86	0.57
2:H:207:GLU:O	2:H:240:LEU:HA	2.06	0.56
2:B:303:ASN:OD1	2:B:304:SER:N	2.38	0.56
1:A:34:PHE:HB2	1:A:43:GLN:O	2.06	0.56
2:D:241:HIS:ND1	2:D:297:VAL:HG22	2.20	0.55
1:C:2:SER:O	1:C:6:GLU:HG3	2.07	0.55
1:A:138:SER:HA	1:A:141:THR:HG22	1.89	0.55
1:C:81:ALA:O	1:C:85:VAL:HG23	2.07	0.55
2:F:264:TYR:CD1	2:F:271:LEU:HB3	2.43	0.54
2:H:224:TYR:N	2:H:316:PHE:O	2.39	0.54
1:G:30:ARG:HA	1:G:142:ILE:HD11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:PRO:CG	1:A:155:GLN:HE21	2.21	0.53
1:E:97:ALA:O	1:E:101:ALA:HB3	2.09	0.53
1:C:39:ILE:HD11	1:C:154:ALA:HB1	1.90	0.52
1:A:55:VAL:HA	1:A:61:MET:HA	1.92	0.52
1:C:6:GLU:O	1:C:10:THR:HB	2.09	0.52
2:F:275:GLU:HB3	2:F:289:ILE:HD11	1.92	0.52
1:C:34:PHE:HB3	1:C:39:ILE:HD13	1.91	0.51
2:B:212:THR:CG2	2:B:244:ILE:HG23	2.39	0.51
2:D:292:ASP:O	2:D:296:TYR:OH	2.13	0.50
2:B:244:ILE:O	2:B:293:ALA:HA	2.12	0.50
1:E:12:LEU:HD22	1:E:172:LEU:HD22	1.93	0.50
2:D:261:PHE:CE1	2:D:277:SER:HB3	2.46	0.50
1:A:57:SER:O	1:A:58:THR:OG1	2.29	0.49
1:C:13:ALA:HB1	1:C:124:PHE:CD1	2.48	0.49
1:E:28:MET:HB3	1:E:46:TRP:NE1	2.26	0.49
1:E:49:LEU:CD2	1:E:73:PRO:HG2	2.41	0.49
1:G:3:MET:HE1	1:G:6:GLU:OE2	2.13	0.49
2:B:205:ALA:CB	2:B:238:LEU:HA	2.21	0.48
2:B:212:THR:HG21	2:B:246:ALA:HB3	1.95	0.48
2:B:260:ASP:OD2	2:B:303:ASN:HB3	2.13	0.48
2:D:257:LYS:HD2	2:D:281:GLY:C	2.38	0.48
2:H:218:ASN:ND2	2:H:223:LEU:O	2.47	0.48
2:F:258:ILE:O	2:F:258:ILE:HG22	2.14	0.47
2:B:298:LEU:HD23	2:B:300:MET:HE2	1.96	0.47
1:A:49:LEU:HD21	1:A:80:ARG:HA	1.97	0.47
1:G:24:CYS:SG	1:G:83:ILE:HG21	2.54	0.47
1:E:102:GLN:HE22	1:G:31:VAL:HG21	1.77	0.47
1:G:96:VAL:O	1:G:116:ILE:HD13	2.15	0.47
2:D:243:THR:OG1	2:D:295:GLN:NE2	2.47	0.47
1:A:23:CYS:SG	1:A:166:GLY:N	2.88	0.47
1:E:6:GLU:OE1	1:G:159:MET:HE1	2.15	0.47
1:E:40:ILE:HD12	2:F:317:GLN:HB3	1.97	0.47
1:C:99:VAL:HG12	1:C:99:VAL:O	2.15	0.47
2:B:214:ALA:HB1	2:B:224:TYR:CE2	2.50	0.47
2:D:300:MET:HE1	2:D:314:ILE:HG13	1.97	0.46
2:D:203:ALA:N	2:D:236:GLN:OE1	2.48	0.46
1:C:29:TRP:CZ2	1:C:83:ILE:HD13	2.50	0.46
1:G:152:PRO:HB3	2:H:256:SER:HA	1.98	0.46
2:B:205:ALA:HB1	2:B:238:LEU:CD1	2.45	0.46
2:F:262:ASN:HD22	2:F:276:GLN:NE2	2.14	0.46
1:A:34:PHE:C	1:A:39:ILE:HD11	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:SER:HA	1:A:167:TRP:HH2	1.82	0.45
1:A:28:MET:HE2	1:C:4:GLY:HA2	1.99	0.45
1:C:19:CYS:O	1:C:22:VAL:N	2.49	0.45
1:C:19:CYS:HB3	1:C:169:ALA:HB2	1.98	0.45
1:A:53:CYS:HA	1:A:63:CYS:HA	1.98	0.45
1:C:150:LEU:HD21	2:D:306:TYR:CE2	2.52	0.45
1:G:10:THR:HA	1:G:13:ALA:HB3	2.00	0.44
2:D:254:LEU:HB3	2:D:315:LEU:HB3	1.99	0.44
1:A:89:LEU:HD21	1:A:126:LEU:HD23	1.99	0.44
1:C:51:MET:HG2	1:C:65:MET:HG2	1.98	0.44
1:A:149:PRO:HD2	2:B:310:TYR:CD2	2.53	0.43
1:C:99:VAL:CG1	1:C:103:ALA:HB2	2.48	0.43
2:B:291:LEU:HD22	2:B:296:TYR:CE2	2.53	0.43
1:C:101:ALA:O	1:C:105:ASN:CG	2.61	0.43
1:E:11:SER:HB3	1:G:167:TRP:CE3	2.53	0.43
1:E:128:ALA:HB2	1:E:173:GLN:HB3	1.99	0.43
2:H:204:ALA:CB	2:H:237:LYS:HG2	2.47	0.43
2:F:258:ILE:HG21	2:F:304:SER:HB3	2.00	0.43
1:G:132:LEU:CD2	1:G:170:ALA:HB1	2.49	0.43
2:D:250:LYS:HA	2:D:290:SER:HA	2.00	0.43
1:E:49:LEU:HD21	1:E:73:PRO:CB	2.46	0.43
2:F:252:ARG:HG3	2:F:288:ASP:HA	2.01	0.43
1:A:44:ILE:HB	1:A:55:VAL:CG1	2.49	0.43
1:C:113:LYS:HA	1:C:116:ILE:HG22	2.01	0.42
1:E:28:MET:HB3	1:E:46:TRP:CD1	2.55	0.42
2:D:262:ASN:HB2	2:D:299:VAL:HB	2.01	0.42
2:H:254:LEU:HD13	2:H:315:LEU:HD23	2.02	0.42
1:E:152:PRO:HG2	1:E:155:GLN:NE2	2.35	0.42
1:E:49:LEU:HD23	1:E:73:PRO:CG	2.48	0.42
1:E:152:PRO:HD3	2:F:313:ALA:HB3	2.02	0.42
1:E:49:LEU:CD2	1:E:73:PRO:CG	2.98	0.42
1:G:157:ARG:HD3	2:H:227:ARG:NH2	2.34	0.42
1:G:153:GLU:N	2:H:284:ASP:OD2	2.53	0.42
1:E:1:MET:HE3	1:E:4:GLY:HA3	2.02	0.41
1:E:150:LEU:HB3	2:F:312:TYR:HA	2.03	0.41
2:H:234:TRP:CG	2:H:305:SER:HA	2.56	0.41
1:C:23:CYS:SG	1:C:24:CYS:N	2.92	0.41
1:C:142:ILE:HG22	1:C:142:ILE:O	2.21	0.41
1:E:1:MET:HE3	1:E:4:GLY:CA	2.51	0.41
1:G:120:ALA:O	1:G:124:PHE:HB2	2.21	0.41
1:A:152:PRO:HG3	1:A:155:GLN:HE21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:GLY:O	1:C:122:VAL:C	2.63	0.41
1:E:151:VAL:HA	2:F:313:ALA:HB3	2.02	0.41
1:G:9:GLY:HA3	1:G:179:LEU:HD22	2.02	0.41
2:D:257:LYS:HG2	2:D:283:LYS:C	2.45	0.41
1:G:96:VAL:CG1	1:G:116:ILE:O	2.69	0.41
2:B:310:TYR:HB3	2:B:311:PRO:HD2	2.03	0.41
1:C:17:TRP:HD1	1:C:90:ALA:HB3	1.85	0.41
1:C:100:GLY:HA2	1:C:116:ILE:HD13	2.03	0.41
1:E:1:MET:HG2	1:E:4:GLY:HA3	2.02	0.41
2:B:255:ALA:HB2	2:B:314:ILE:CD1	2.50	0.41
2:F:242:LEU:CB	2:F:296:TYR:HB2	2.49	0.41
2:B:255:ALA:O	2:B:284:ASP:OD1	2.38	0.40
2:B:260:ASP:HB3	2:B:278:LEU:CD2	2.51	0.40
1:A:14:VAL:HG22	1:A:94:LEU:HD11	2.02	0.40
1:A:30:ARG:HG3	1:A:142:ILE:HD12	2.03	0.40
1:A:34:PHE:CD2	2:B:223:LEU:HD21	2.57	0.40
1:A:39:ILE:HG22	2:B:317:GLN:NE2	2.36	0.40
1:C:5:LEU:O	1:C:6:GLU:C	2.64	0.40
2:D:252:ARG:HG2	2:D:288:ASP:OD1	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	A	182/190 (96%)	178 (98%)	4 (2%)	0	100	100
1	C	184/190 (97%)	181 (98%)	3 (2%)	0	100	100
1	E	168/190 (88%)	165 (98%)	3 (2%)	0	100	100
1	G	163/190 (86%)	159 (98%)	4 (2%)	0	100	100
2	B	115/119 (97%)	113 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	115/119 (97%)	112 (97%)	3 (3%)	0	100	100
2	F	115/119 (97%)	114 (99%)	1 (1%)	0	100	100
2	H	115/119 (97%)	114 (99%)	1 (1%)	0	100	100
All	All	1157/1236 (94%)	1136 (98%)	21 (2%)	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	135/143 (94%)	135 (100%)	0	100	100
1	C	138/143 (96%)	138 (100%)	0	100	100
1	E	126/143 (88%)	126 (100%)	0	100	100
1	G	121/143 (85%)	121 (100%)	0	100	100
2	B	99/102 (97%)	99 (100%)	0	100	100
2	D	101/102 (99%)	101 (100%)	0	100	100
2	F	100/102 (98%)	100 (100%)	0	100	100
2	H	101/102 (99%)	101 (100%)	0	100	100
All	All	921/980 (94%)	921 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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	43	GLN
1	A	56	GLN
1	A	155	GLN
1	C	56	GLN
1	C	62	GLN

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Mol	Chain	Res	Type
1	E	102	GLN
1	G	74	GLN
1	G	140	ASN
1	G	173	GLN
2	B	218	ASN
2	B	236	GLN
2	B	266	ASN
2	B	285	HIS
2	D	218	ASN
2	D	266	ASN
2	D	295	GLN
2	F	276	GLN
2	F	317	GLN
2	H	216	ASN
2	H	218	ASN
2	H	249	GLN
2	H	295	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

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	184/190 (96%)	1.48	56 (30%) 1 3	53, 91, 142, 171	0
1	C	186/190 (97%)	1.50	48 (25%) 1 4	55, 97, 167, 258	0
1	E	174/190 (91%)	2.40	73 (41%) 0 1	84, 147, 232, 357	0
1	G	169/190 (88%)	2.06	59 (34%) 1 2	87, 149, 208, 247	0
2	B	117/119 (98%)	0.60	15 (12%) 7 11	42, 83, 133, 192	0
2	D	117/119 (98%)	0.94	21 (17%) 3 6	51, 91, 130, 183	0
2	F	117/119 (98%)	1.22	28 (23%) 2 4	86, 138, 198, 228	0
2	H	117/119 (98%)	1.07	23 (19%) 3 5	73, 121, 154, 182	0
All	All	1181/1236 (95%)	1.50	323 (27%) 1 3	42, 115, 193, 357	0

All (323) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	159	MET	16.8
1	G	42	ALA	16.3
1	G	75	ASP	15.9
1	E	92	PHE	14.8
1	C	158	GLU	14.8
1	E	159	MET	13.5
1	G	47	GLU	13.0
1	C	160	GLY	12.6
1	G	30	ARG	12.6
2	F	205	ALA	10.9
1	E	48	GLY	10.2
2	F	250	LYS	10.1
1	C	161	ALA	8.8
1	E	164	TYR	8.7
1	E	47	GLU	8.6
2	H	203	ALA	8.5

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Mol	Chain	Res	Type	RSRZ
1	E	99	VAL	8.5
1	E	160	GLY	8.5
1	G	49	LEU	8.3
1	C	31	VAL	8.2
1	E	136	SER	8.2
1	A	158	GLU	7.9
1	E	103	ALA	7.8
1	G	144	ARG	7.8
1	C	163	LEU	7.7
2	F	204	ALA	7.6
1	G	50	TRP	7.6
1	A	102	GLN	7.5
1	E	27	PRO	7.4
1	A	104	THR	7.2
1	E	46	TRP	7.2
1	A	109	ASP	7.1
1	E	30	ARG	7.0
1	C	157	ARG	6.9
1	C	164	TYR	6.9
1	C	1	MET	6.9
1	G	41	THR	6.8
1	E	1	MET	6.7
1	E	158	GLU	6.7
1	C	70	LEU	6.7
2	B	204	ALA	6.7
1	E	53	CYS	6.5
1	C	167	TRP	6.5
1	G	48	GLY	6.5
1	A	98	LEU	6.5
1	G	137	TRP	6.4
1	E	140	ASN	6.4
1	A	164	TYR	6.3
1	C	28	MET	6.3
1	A	103	ALA	6.2
1	G	76	LEU	6.2
2	D	213	ASP	6.2
1	C	30	ARG	6.2
1	A	110	GLU	6.1
1	A	108	GLN	6.1
1	E	52	ASN	6.0
2	D	267	ASN	6.0
2	H	224	TYR	5.9

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Mol	Chain	Res	Type	RSRZ
2	F	238	LEU	5.9
2	F	206	THR	5.9
1	E	28	MET	5.8
2	B	282	VAL	5.8
1	E	31	VAL	5.8
1	A	153	GLU	5.7
1	E	137	TRP	5.7
1	E	139	ALA	5.7
2	H	204	ALA	5.7
1	A	111	THR	5.6
1	A	99	VAL	5.6
1	A	159	MET	5.5
1	E	161	ALA	5.4
1	A	38	SER	5.4
1	C	139	ALA	5.4
1	C	5	LEU	5.2
1	E	143	ILE	5.2
1	C	75	ASP	5.1
1	A	106	ALA	5.0
2	D	268	PHE	5.0
1	A	147	TYR	5.0
2	D	210	ASN	4.9
2	F	239	ASN	4.9
1	E	29	TRP	4.9
1	G	147	TYR	4.9
1	G	141	THR	4.9
2	B	203	ALA	4.9
1	G	10	THR	4.8
1	E	88	LEU	4.8
1	G	40	ILE	4.8
1	E	167	TRP	4.8
1	C	138	SER	4.8
1	A	105	ASN	4.8
2	F	203	ALA	4.7
2	H	269	ASN	4.7
1	E	138	SER	4.7
1	C	29	TRP	4.7
1	E	63	CYS	4.7
1	A	154	ALA	4.7
2	D	270	ASN	4.7
1	E	124	PHE	4.6
1	G	80	ARG	4.6

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Mol	Chain	Res	Type	RSRZ
2	D	208	ARG	4.6
2	D	229	SER	4.5
1	E	83	ILE	4.5
1	G	29	TRP	4.5
2	F	220	ALA	4.4
1	A	74	GLN	4.4
1	C	118	ILE	4.4
2	F	251	TYR	4.3
1	G	140	ASN	4.3
2	D	209	LEU	4.3
2	F	237	LYS	4.3
1	G	7	ILE	4.2
2	F	207	GLU	4.2
2	H	237	LYS	4.2
1	E	133	VAL	4.1
1	C	155	GLN	4.1
1	E	142	ILE	4.1
1	E	163	LEU	4.0
1	C	144	ARG	4.0
1	A	37	SER	3.9
1	E	131	THR	3.9
1	G	131	THR	3.9
1	E	76	LEU	3.9
1	C	162	GLY	3.9
2	H	283	LYS	3.8
1	A	101	ALA	3.8
2	F	299	VAL	3.8
1	G	46	TRP	3.8
2	H	236	GLN	3.7
1	G	88	LEU	3.7
1	G	74	GLN	3.7
2	B	217	SER	3.7
2	B	276	GLN	3.7
2	F	319	PHE	3.7
1	G	120	ALA	3.6
1	E	105	ASN	3.6
1	A	50	TRP	3.6
1	C	142	ILE	3.6
1	A	100	GLY	3.6
1	A	64	LYS	3.6
1	C	135	VAL	3.6
2	F	290	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	74	GLN	3.6
1	E	98	LEU	3.6
1	E	13	ALA	3.5
1	G	5	LEU	3.5
1	E	116	ILE	3.5
2	H	225	ASP	3.5
1	E	87	ILE	3.5
1	A	36	GLY	3.5
1	A	7	ILE	3.4
1	E	86	SER	3.4
2	F	300	MET	3.4
1	E	45	THR	3.4
2	H	273	LYS	3.4
2	F	289	ILE	3.3
1	E	95	LEU	3.3
1	C	181	ALA	3.3
1	E	114	ALA	3.3
2	D	243	THR	3.3
1	E	127	ALA	3.3
1	E	100	GLY	3.3
1	C	103	ALA	3.3
2	B	225	ASP	3.3
1	E	3	MET	3.3
1	A	156	LYS	3.3
1	A	143	ILE	3.2
1	E	104	THR	3.2
1	G	110	GLU	3.2
1	G	45	THR	3.2
1	A	161	ALA	3.1
1	A	155	GLN	3.1
1	E	120	ALA	3.1
1	G	8	THR	3.1
1	G	56	GLN	3.1
1	C	46	TRP	3.1
2	F	307	SER	3.0
1	E	93	GLY	3.0
1	E	84	VAL	3.0
1	E	82	LEU	2.9
2	H	227	ARG	2.9
2	D	203	ALA	2.9
1	E	123	LEU	2.9
1	G	157	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	G	20	THR	2.9
2	D	230	ASN	2.9
2	D	269	ASN	2.9
2	D	271	LEU	2.9
2	F	310	TYR	2.9
1	E	6	GLU	2.9
1	E	108	GLN	2.9
2	H	229	SER	2.9
1	C	156	LYS	2.9
1	A	160	GLY	2.9
1	A	127	ALA	2.8
1	E	91	ALA	2.8
1	E	112	ALA	2.8
1	C	119	VAL	2.8
1	C	183	SER	2.8
2	D	241	HIS	2.8
2	F	263	ILE	2.8
1	G	43	GLN	2.8
1	C	61	MET	2.8
1	C	179	LEU	2.8
1	G	77	GLN	2.7
2	D	206	THR	2.7
1	G	89	LEU	2.7
1	C	35	ILE	2.7
2	H	232	TYR	2.7
1	E	96	VAL	2.7
2	H	214	ALA	2.7
1	E	89	LEU	2.7
2	B	236	GLN	2.7
1	E	26	LEU	2.7
1	E	73	PRO	2.7
1	A	128	ALA	2.7
2	F	311	PRO	2.6
1	G	112	ALA	2.6
1	E	51	MET	2.6
1	G	23	CYS	2.6
1	A	35	ILE	2.6
1	A	181	ALA	2.6
1	A	142	ILE	2.6
2	D	259	VAL	2.6
2	F	276	GLN	2.6
1	G	138	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	94	LEU	2.6
2	F	223	LEU	2.6
1	C	146	PHE	2.6
1	E	20	THR	2.5
2	D	212	THR	2.5
2	F	318	LYS	2.5
2	B	247	THR	2.5
1	E	122	VAL	2.5
2	H	218	ASN	2.5
2	B	221	GLY	2.5
2	D	258	ILE	2.5
2	H	228	SER	2.5
1	G	35	ILE	2.5
2	F	288	ASP	2.5
1	E	129	LEU	2.5
1	G	11	SER	2.5
1	E	61	MET	2.5
1	G	66	TYR	2.5
1	C	33	ALA	2.5
1	A	183	SER	2.5
1	A	146	PHE	2.4
1	G	146	PHE	2.4
1	A	90	ALA	2.4
1	G	172	LEU	2.4
1	E	18	LEU	2.4
1	E	90	ALA	2.4
1	E	162	GLY	2.4
1	G	159	MET	2.4
2	H	223	LEU	2.4
1	G	170	ALA	2.4
1	G	83	ILE	2.4
1	G	87	ILE	2.4
1	C	182	ALA	2.4
2	H	301	LYS	2.4
1	A	177	GLY	2.4
1	E	173	GLN	2.3
2	H	257	LYS	2.4
1	C	101	ALA	2.3
2	F	222	ASN	2.3
1	C	41	THR	2.3
1	A	182	ALA	2.3
1	A	173	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	242	LEU	2.3
1	G	93	GLY	2.3
2	B	307	SER	2.3
2	H	231	SER	2.3
1	C	107	VAL	2.3
1	G	123	LEU	2.3
1	G	135	VAL	2.3
2	H	219	PRO	2.3
2	B	295	GLN	2.3
1	C	32	SER	2.3
2	F	229	SER	2.3
1	A	121	GLY	2.3
1	A	145	ASP	2.3
1	G	179	LEU	2.2
1	A	11	SER	2.2
1	A	86	SER	2.2
1	C	122	VAL	2.2
1	G	109	ASP	2.2
1	G	44	ILE	2.2
1	A	157	ARG	2.2
1	A	174	LEU	2.2
1	C	86	SER	2.2
1	C	153	GLU	2.2
2	F	245	THR	2.2
2	D	266	ASN	2.2
2	H	284	ASP	2.2
1	G	167	TRP	2.2
1	C	0	SER	2.2
1	A	70	LEU	2.2
2	B	259	VAL	2.2
1	G	4	GLY	2.2
1	A	51	MET	2.1
1	A	71	ALA	2.1
1	G	57	SER	2.1
1	C	36	GLY	2.1
1	G	166	GLY	2.1
2	B	219	PRO	2.1
1	A	125	LEU	2.1
1	E	17	TRP	2.1
2	F	232	TYR	2.1
1	A	89	LEU	2.1
1	A	97	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	42	ALA	2.1
2	D	288	ASP	2.1
1	A	42	ALA	2.1
1	G	33	ALA	2.1
2	H	217	SER	2.1
2	H	282	VAL	2.1
2	B	308	GLY	2.0
2	B	301	LYS	2.0
1	C	82	LEU	2.0
1	G	62	GLN	2.0
1	A	49	LEU	2.0
1	C	113	LYS	2.0
1	G	113	LYS	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.