



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 13, 2025 – 10:12 AM EDT

PDB ID : 9PZI / pdb\_00009pzi  
Title : Crystal Structure of synthetic antibody COP-2 in complex with the C-terminal domain of Clostridium perfringens enterotoxin  
Authors : Vecchio, A.J.; Ogbu, C.P.; Kapoor, S.  
Deposited on : 2025-08-11  
Resolution : 2.50 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](mailto: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>.

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

MolProbity : 4-5-2 with Phenix2.0rc1  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

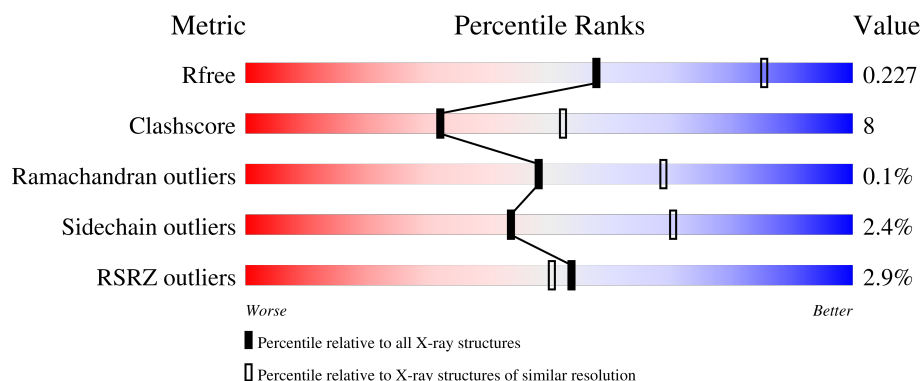
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	164625	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

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  $\geq 3$ , 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	239	
1	C	239	
1	E	239	
2	B	260	
2	D	260	

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Mol	Chain	Length	Quality of chain
2	F	260	<div><div></div><div>6%</div><div>73%</div><div>11%</div><div>•</div><div>15%</div></div>
3	G	134	<div><div></div><div>%</div><div>82%</div><div>9%</div><div>9%</div></div>
3	H	134	<div><div></div><div>2%</div><div>85%</div><div>8%</div><div>•</div><div>6%</div></div>
3	I	134	<div><div></div><div>%</div><div>86%</div><div>6%</div><div>8%</div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 25529 atoms, of which 12397 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 COP-2 Light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	C	212	Total	C	H	N	O	S	0	0	0
			3210	1019	1583	273	330	5			
1	A	213	Total	C	H	N	O	S	0	0	0
			3220	1022	1588	274	331	5			
1	E	213	Total	C	H	N	O	S	0	0	0
			3220	1022	1588	274	331	5			

- Molecule 2 is a protein called COP-2 Heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	D	221	Total	C	H	N	O	S	0	0	0
			3257	1054	1595	274	329	5			
2	B	220	Total	C	H	N	O	S	0	0	0
			3246	1051	1590	273	327	5			
2	F	221	Total	C	H	N	O	S	0	0	0
			3209	1044	1561	272	327	5			

- Molecule 3 is a protein called Heat-labile enterotoxin B chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	G	122	Total	C	H	N	O	S	0	0	0
			1913	618	945	162	187	1			
3	I	123	Total	C	H	N	O	S	0	0	0
			1935	625	958	163	188	1			
3	H	126	Total	C	H	N	O	S	0	1	0
			1996	644	989	168	194	1			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	191	MET	-	initiating methionine	UNP P01558
G	320	GLY	-	expression tag	UNP P01558

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Chain	Residue	Modelled	Actual	Comment	Reference
G	321	LEU	-	expression tag	UNP P01558
G	322	VAL	-	expression tag	UNP P01558
G	323	PRO	-	expression tag	UNP P01558
G	324	ARG	-	expression tag	UNP P01558
I	191	MET	-	initiating methionine	UNP P01558
I	320	GLY	-	expression tag	UNP P01558
I	321	LEU	-	expression tag	UNP P01558
I	322	VAL	-	expression tag	UNP P01558
I	323	PRO	-	expression tag	UNP P01558
I	324	ARG	-	expression tag	UNP P01558
H	191	MET	-	initiating methionine	UNP P01558
H	320	GLY	-	expression tag	UNP P01558
H	321	LEU	-	expression tag	UNP P01558
H	322	VAL	-	expression tag	UNP P01558
H	323	PRO	-	expression tag	UNP P01558
H	324	ARG	-	expression tag	UNP P01558

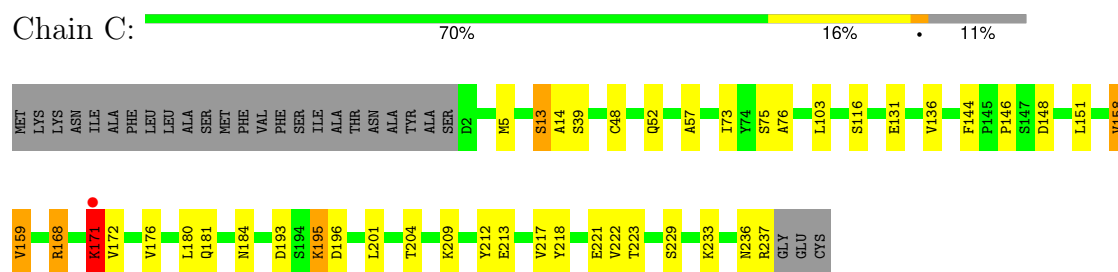
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	41	Total O 41 41	0	0
4	D	41	Total O 41 41	0	0
4	A	49	Total O 49 49	0	0
4	B	18	Total O 18 18	0	0
4	E	39	Total O 39 39	0	0
4	F	32	Total O 32 32	0	0
4	G	41	Total O 41 41	0	0
4	I	23	Total O 23 23	0	0
4	H	39	Total O 39 39	0	0

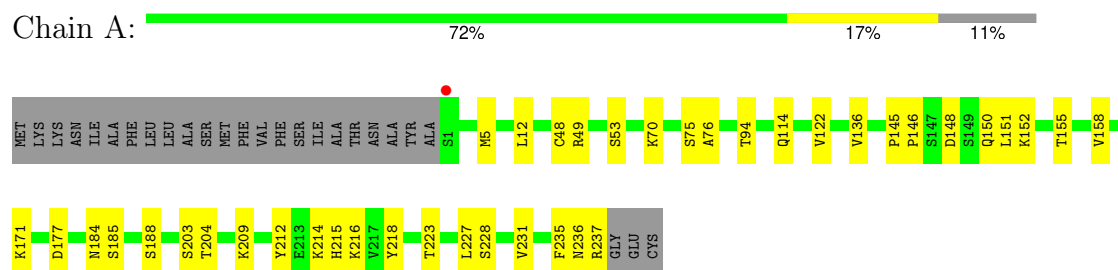
### 3 Residue-property plots

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

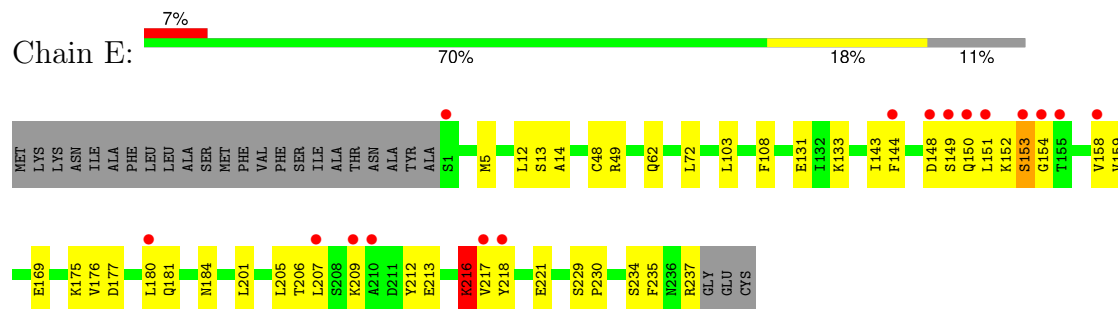
- Molecule 1: COP-2 Light chain



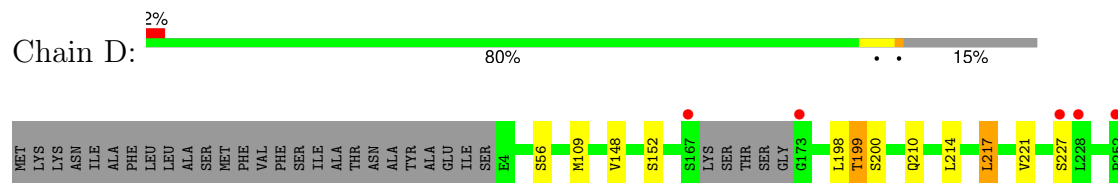
- Molecule 1: COP-2 Light chain



- Molecule 1: COP-2 Light chain



- Molecule 2: COP-2 Heavy chain



LYS  
SER  
CYS  
ASP  
LYS  
THR  
HIS  
THR

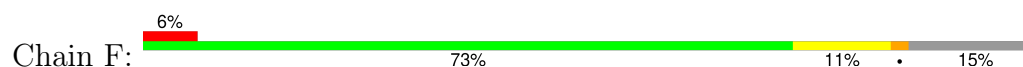
• Molecule 2: COP-2 Heavy chain



MET LYS LYS ASN ILE ALA PHE LEU LEU ALA SER MET PHE VAL PHE SER SER ILE ALA THR ASN ALA TYR TYR ALA GLU ILE ILE SER E4 V5 Q6 L7 S10 L14 R45 L46 S47 C48 S51 G68 K69 I77 T84 S97 M109 N110 S111 L112 R113 D116 Y141

V148 T149 S152 K156 G157 P158 S166 SER LYS SER THR SER GLY G173 K182 P188 L198 Q210 G213 L214 L217 V221 S226 Q231 T232 K240 P241 T244 K248 K249 P252 LYS SER CYS ASP LYS THR HIS THR

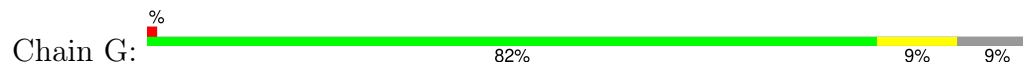
• Molecule 2: COP-2 Heavy chain



MET LYS LYS ASN ILE ALA PHE LEU LEU ALA SER MET PHE VAL PHE SER SER ILE ALA THR ASN ALA TYR TYR ALA GLU ILE ILE SER E4 V5 Q6 V38 Q39 P40 S43 S51 M109 L112 E115 V148 S152 K156 S159 V160 F161 P162 L163 A164 P165 S166 LYS

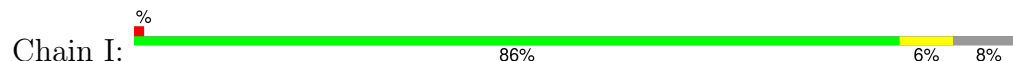
SER THR SER ASP GLY G173 G178 K182 D183 Y184 V189 S192 L198 T199 S200 L214 Y215 S216 L217 V221 S227 L228 Q229 T230 Q231 T232 C235 N236 D247 K248 K249 V250 E251 P252 LYS SER CYS ASP LYS THR HIS THR

• Molecule 3: Heat-labile enterotoxin B chain



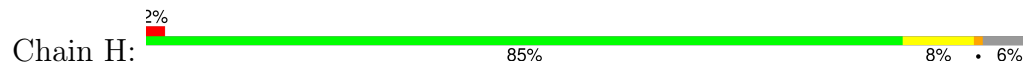
MET SER THR ASP ILE ILE LYS GLU D201 R208 L209 L223 L242 I258 I263 Y264 S265 N269 N270 L271 L274 E275 V322 PRO ARG

• Molecule 3: Heat-labile enterotoxin B chain



MET SER THR ASP ILE ILE LYS GLU T199 S229 N230 S231 K237 L242 K283 M300 N309 L321 VAL PRO ARG

• Molecule 3: Heat-labile enterotoxin B chain



MET SER THR ASP ILE ILE LYS GLU K197 E198 T199 L200 T206 L215 P219 A220 Q221 K237 N267 F268 N269 V322 PRO ARG

## 4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	111.47Å 198.52Å 115.80Å 90.00° 109.72° 90.00°	Depositor
Resolution (Å)	29.74 – 2.50 29.74 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.2 (29.74-2.50) 99.1 (29.74-2.50)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.81 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, $R_{free}$	0.178 , 0.225 0.181 , 0.227	Depositor DCC
$R_{free}$ test set	3984 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.0	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 48.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.008 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	25529	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.56	0/1668	0.75	2/2267 (0.1%)
1	C	0.88	6/1663 (0.4%)	0.95	10/2260 (0.4%)
1	E	0.64	1/1668 (0.1%)	0.76	0/2267
2	B	0.66	3/1701 (0.2%)	0.88	10/2323 (0.4%)
2	D	0.57	0/1707	0.74	2/2331 (0.1%)
2	F	0.59	0/1693	0.88	7/2315 (0.3%)
3	G	0.61	0/989	0.74	0/1345
3	H	0.58	0/1031	0.77	0/1401
3	I	0.59	0/998	0.71	0/1357
All	All	0.65	10/13118 (0.1%)	0.81	31/17866 (0.2%)

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	C	0	1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	171	LYS	CE-NZ	12.57	1.87	1.49
1	C	171	LYS	CD-CE	12.54	1.90	1.52
2	B	232	THR	CB-CG2	10.64	1.87	1.52
1	C	195	LYS	CD-CE	10.08	1.82	1.52
1	C	195	LYS	CE-NZ	8.99	1.76	1.49
1	C	171	LYS	CG-CD	8.89	1.79	1.52
1	E	216	LYS	CA-C	-8.53	1.47	1.52
2	B	69	LYS	CD-CE	8.06	1.76	1.52
1	C	195	LYS	CG-CD	5.59	1.69	1.52
2	B	69	LYS	CB-CG	5.02	1.67	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	39	GLN	N-CA-CB	11.54	125.71	109.78
1	C	195	LYS	CD-CE-NZ	-10.70	77.67	111.90
2	B	232	THR	OG1-CB-CG2	-9.46	90.39	109.30
2	B	69	LYS	CA-CB-CG	9.28	132.66	114.10
1	C	171	LYS	CD-CE-NZ	-9.12	82.71	111.90
2	B	232	THR	CA-CB-CG2	-8.97	95.25	110.50
1	C	159	VAL	CG1-CB-CG2	8.88	130.34	110.80
2	F	39	GLN	CA-CB-CG	8.64	131.39	114.10
2	B	232	THR	CA-CB-OG1	7.71	121.17	109.60
2	D	227	SER	CB-CA-C	7.53	124.04	110.72
1	C	195	LYS	CG-CD-CE	7.36	128.24	111.30
1	A	228	SER	CB-CA-C	-7.30	96.65	110.67
2	B	232	THR	CA-C-N	-7.29	112.51	122.86
2	B	232	THR	C-N-CA	-7.29	112.51	122.86
1	C	195	LYS	N-CA-C	-7.17	104.52	113.55
1	C	195	LYS	CB-CG-CD	6.74	126.80	111.30
2	F	38	VAL	CA-C-N	-6.68	107.85	121.48
2	F	38	VAL	C-N-CA	-6.68	107.85	121.48
2	F	156	LYS	CA-CB-CG	6.53	127.16	114.10
1	A	228	SER	N-CA-CB	6.10	119.73	110.28
2	B	232	THR	CA-C-O	-6.04	114.52	121.47
1	C	158	VAL	CA-C-N	-5.99	114.61	122.94
1	C	158	VAL	C-N-CA	-5.99	114.61	122.94
2	B	69	LYS	CG-CD-CE	-5.87	97.80	111.30
1	C	171	LYS	CB-CG-CD	5.76	124.55	111.30
2	F	156	LYS	CB-CG-CD	5.75	124.53	111.30
1	C	171	LYS	CA-CB-CG	-5.54	103.03	114.10
2	F	39	GLN	CB-CG-CD	5.52	121.98	112.60
2	D	227	SER	N-CA-C	-5.40	107.00	113.21
2	B	232	THR	CB-CA-C	-5.39	99.54	109.46
2	B	156	LYS	CB-CG-CD	5.35	123.60	111.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	168	ARG	Sidechain

## 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	1632	1588	1588	24	0
1	C	1627	1583	1583	41	0
1	E	1632	1588	1588	41	0
2	B	1656	1590	1589	39	0
2	D	1662	1595	1594	8	0
2	F	1648	1561	1561	31	0
3	G	968	945	945	10	0
3	H	1007	989	992	9	0
3	I	977	958	958	3	0
4	A	49	0	0	3	0
4	B	18	0	0	1	0
4	C	41	0	0	3	0
4	D	41	0	0	1	0
4	E	39	0	0	2	0
4	F	32	0	0	0	0
4	G	41	0	0	0	0
4	H	39	0	0	0	1
4	I	23	0	0	0	0
All	All	13132	12397	12398	198	1

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 (198) 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:69:LYS:CD	2:B:69:LYS:CE	1.76	1.57
1:C:171:LYS:CG	1:C:171:LYS:CD	1.79	1.54
1:C:195:LYS:CD	1:C:195:LYS:CE	1.82	1.52
2:B:232:THR:CB	2:B:232:THR:CG2	1.87	1.50
1:C:171:LYS:CD	1:C:171:LYS:CE	1.90	1.49
1:C:195:LYS:CE	1:C:195:LYS:NZ	1.76	1.44
1:C:171:LYS:CE	1:C:171:LYS:NZ	1.87	1.37
2:B:69:LYS:HB3	2:B:69:LYS:HE2	1.35	1.07
1:C:195:LYS:CD	1:C:195:LYS:NZ	2.25	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:198:LEU:HD21	2:B:221:VAL:HG21	1.45	0.99
2:F:39:GLN:HB3	2:F:40:PRO:CD	1.94	0.97
2:F:39:GLN:HB3	2:F:40:PRO:HD2	1.45	0.97
2:D:198:LEU:HD21	2:D:221:VAL:HG21	1.47	0.96
2:B:232:THR:CG2	2:B:232:THR:CA	2.50	0.88
1:A:227:LEU:HD13	1:A:231:VAL:HG23	1.56	0.87
2:F:4:GLU:N	2:F:4:GLU:OE2	2.09	0.85
2:B:69:LYS:CE	2:B:69:LYS:CG	2.58	0.82
2:F:39:GLN:HG2	2:F:152:SER:HA	1.60	0.81
2:B:248:LYS:HA	2:B:248:LYS:HE2	1.64	0.78
2:F:115:GLU:N	2:F:115:GLU:OE1	2.16	0.78
2:B:69:LYS:CE	2:B:69:LYS:HB3	2.14	0.76
1:A:184:ASN:OD1	4:A:301:HOH:O	2.03	0.76
1:C:171:LYS:CD	1:C:171:LYS:NZ	2.49	0.75
2:B:232:THR:CG2	2:B:232:THR:OG1	2.33	0.75
2:B:69:LYS:HE2	2:B:69:LYS:CB	2.16	0.74
1:C:5:MET:HE3	1:C:48:CYS:SG	2.28	0.73
3:G:269:ASN:HD21	3:H:206:THR:HG21	1.53	0.73
2:B:198:LEU:CD2	2:B:221:VAL:HG21	2.18	0.72
2:F:198:LEU:HD21	2:F:221:VAL:HG21	1.72	0.72
2:B:69:LYS:CD	2:B:69:LYS:NZ	2.51	0.72
1:C:229:SER:HA	2:B:69:LYS:HD3	1.72	0.71
1:A:70:LYS:HE3	4:A:320:HOH:O	1.91	0.71
2:D:109:MET:HE1	2:D:148:VAL:HG21	1.73	0.71
1:A:203:SER:OG	4:A:302:HOH:O	2.04	0.70
1:E:184:ASN:N	1:E:184:ASN:OD1	2.24	0.70
3:H:267[A]:ASN:ND2	3:H:269:ASN:OD1	2.25	0.69
2:F:156:LYS:HG3	2:F:214:LEU:HD21	1.73	0.69
1:C:195:LYS:NZ	1:C:195:LYS:HD2	2.08	0.69
1:A:136:VAL:O	1:E:49:ARG:NH2	2.25	0.69
2:B:46:LEU:HG	2:B:109:MET:HE2	1.75	0.68
1:E:152:LYS:O	1:E:154:GLY:N	2.27	0.68
1:E:213:GLU:HA	1:E:237:ARG:NH1	2.11	0.66
1:C:159:VAL:CG2	1:C:204:THR:OG1	2.45	0.65
2:F:183:ASP:CA	2:F:214:LEU:HD23	2.27	0.65
1:E:5:MET:HE3	1:E:48:CYS:SG	2.38	0.64
2:F:183:ASP:HB3	2:F:214:LEU:HD23	1.80	0.63
1:E:108:PHE:O	4:E:301:HOH:O	2.15	0.63
2:B:214:LEU:N	2:B:214:LEU:HD12	2.13	0.62
2:B:232:THR:CG2	2:B:232:THR:HA	2.30	0.62
2:F:109:MET:HB3	2:F:112:LEU:HD21	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:69:LYS:CE	2:B:69:LYS:CB	2.77	0.61
1:C:217:VAL:HG22	1:C:236:ASN:OD1	2.00	0.61
2:F:183:ASP:C	2:F:214:LEU:HD23	2.26	0.61
1:E:213:GLU:O	1:E:237:ARG:NH1	2.34	0.61
1:E:177:ASP:HA	1:E:217:VAL:CG2	2.30	0.60
3:H:215:LEU:O	3:H:221:GLY:HA2	2.00	0.60
1:A:215:HIS:O	1:A:237:ARG:NE	2.31	0.60
1:A:214:LYS:HD3	1:A:215:HIS:NE2	2.17	0.60
2:F:184:TYR:CE1	2:F:189:VAL:HG21	2.37	0.59
1:E:169:GLU:OE1	1:E:169:GLU:N	2.27	0.59
2:B:109:MET:HE1	2:B:148:VAL:HG21	1.84	0.59
1:C:209:LYS:O	1:C:213:GLU:HG3	2.04	0.58
1:C:171:LYS:O	1:C:222:VAL:HA	2.03	0.58
2:F:192:SER:HB2	2:F:236:ASN:HB2	1.87	0.57
1:A:5:MET:HE3	1:A:48:CYS:SG	2.45	0.57
3:I:199:ILE:HG22	3:I:199:ILE:O	2.04	0.57
2:D:198:LEU:CD2	2:D:221:VAL:HG21	2.30	0.56
1:C:180:LEU:HD23	1:C:181:GLN:C	2.29	0.56
1:E:148:ASP:C	1:E:150:GLN:H	2.12	0.56
1:E:184:ASN:ND2	1:E:205:LEU:HD11	2.20	0.56
1:C:151:LEU:HD22	1:C:209:LYS:HG3	1.87	0.56
3:I:231:SER:HB3	3:I:309:ASN:HB3	1.88	0.55
3:H:322:VAL:HG22	3:H:322:VAL:O	2.05	0.55
2:D:56:SER:OG	4:D:301:HOH:O	2.18	0.55
1:C:180:LEU:HD23	1:C:180:LEU:C	2.32	0.55
1:A:227:LEU:HD13	1:A:231:VAL:CG2	2.33	0.55
1:E:234:SER:O	4:E:302:HOH:O	2.18	0.55
1:C:195:LYS:HD2	1:C:195:LYS:HZ2	1.72	0.55
1:A:177:ASP:OD2	1:A:215:HIS:ND1	2.40	0.54
1:C:146:PRO:HD3	1:C:158:VAL:HG22	1.88	0.54
2:B:68:GLY:O	2:B:69:LYS:HB3	2.09	0.53
1:A:75:SER:O	1:A:76:ALA:HB3	2.08	0.53
3:H:199:ILE:HG22	3:H:199:ILE:O	2.09	0.53
2:F:182:LYS:HE3	2:F:183:ASP:OD2	2.10	0.52
2:B:217:LEU:C	2:B:217:LEU:HD12	2.35	0.52
1:E:144:PHE:HB2	1:E:159:VAL:CG1	2.39	0.52
1:A:12:LEU:HD12	1:A:12:LEU:C	2.35	0.52
1:A:148:ASP:O	1:A:152:LYS:HD3	2.10	0.52
1:E:201:LEU:C	1:E:201:LEU:HD23	2.35	0.52
2:F:183:ASP:CB	2:F:214:LEU:HD23	2.40	0.52
3:G:201:ASP:N	3:G:201:ASP:OD1	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:PRO:HD3	1:A:158:VAL:HG22	1.93	0.50
1:E:153:SER:HB2	1:E:209:LYS:HD3	1.94	0.50
2:B:231:GLN:OE1	2:B:232:THR:N	2.44	0.50
2:F:235:CYS:O	2:F:247:ASP:HA	2.12	0.50
1:C:144:PHE:HB2	1:C:159:VAL:HG12	1.94	0.49
2:B:232:THR:HG22	2:B:249:LYS:NZ	2.27	0.49
1:C:176:VAL:HG23	1:C:181:GLN:OE1	2.12	0.49
1:E:13:SER:HB3	1:E:133:LYS:HG3	1.95	0.49
1:E:150:GLN:O	1:E:153:SER:HB3	2.11	0.49
1:E:175:LYS:NZ	1:E:221:GLU:OE1	2.42	0.49
1:E:153:SER:O	1:E:154:GLY:C	2.54	0.49
3:H:267[A]:ASN:CG	3:H:269:ASN:OD1	2.55	0.49
2:F:183:ASP:HB3	2:F:214:LEU:CD2	2.43	0.48
1:E:184:ASN:HD22	1:E:207:LEU:HD21	1.78	0.48
3:G:208:ARG:HG3	3:G:208:ARG:NH1	2.28	0.48
1:E:144:PHE:HB2	1:E:159:VAL:HG13	1.95	0.48
3:G:274:LEU:O	3:G:275:GLU:HG2	2.14	0.48
1:E:150:GLN:O	1:E:153:SER:N	2.47	0.47
2:F:217:LEU:C	2:F:217:LEU:HD12	2.39	0.47
1:C:14:ALA:HB3	1:C:103:LEU:HD22	1.96	0.47
1:C:168:ARG:NH2	4:C:306:HOH:O	2.47	0.47
1:C:180:LEU:HD23	1:C:181:GLN:O	2.14	0.47
1:C:13:SER:HA	1:C:131:GLU:O	2.15	0.47
2:B:45:ARG:NH1	4:B:301:HOH:O	2.12	0.47
2:B:156:LYS:HG3	2:B:157:GLY:N	2.30	0.47
3:G:209:LEU:HD23	3:G:242:LEU:HD21	1.96	0.47
1:C:159:VAL:HG23	1:C:204:THR:OG1	2.16	0.46
1:E:218:TYR:HB2	1:E:235:PHE:CE2	2.50	0.46
3:G:258:ILE:HG22	3:G:258:ILE:O	2.14	0.46
3:H:197:LYS:CD	3:H:200:LEU:HD23	2.46	0.46
1:A:185:SER:HA	1:A:204:THR:O	2.16	0.46
1:E:176:VAL:HG21	1:E:181:GLN:OE1	2.16	0.46
2:F:198:LEU:CD2	2:F:221:VAL:HG21	2.45	0.46
2:F:192:SER:HB2	2:F:236:ASN:OD1	2.16	0.45
1:C:172:VAL:HG22	1:C:222:VAL:HG22	1.98	0.45
1:E:14:ALA:HB3	1:E:103:LEU:HD22	1.99	0.45
2:B:46:LEU:CG	2:B:109:MET:HE2	2.44	0.45
2:B:214:LEU:N	2:B:214:LEU:CD1	2.78	0.45
1:C:159:VAL:HG23	1:C:204:THR:HG23	1.99	0.45
1:E:181:GLN:HB3	1:E:184:ASN:HD21	1.82	0.45
1:C:184:ASN:N	1:C:184:ASN:OD1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:14:LEU:HD12	2:B:149:THR:O	2.17	0.44
2:D:199:THR:CG2	2:D:200:SER:N	2.80	0.44
2:B:7:LEU:HD22	2:B:48:CYS:SG	2.58	0.44
2:B:232:THR:HG22	2:B:249:LYS:HZ1	1.83	0.44
2:F:182:LYS:HE3	2:F:183:ASP:CG	2.42	0.44
1:C:212:TYR:HA	1:C:218:TYR:OH	2.17	0.44
1:C:236:ASN:O	1:C:237:ARG:HB2	2.17	0.44
3:H:197:LYS:HB3	3:H:200:LEU:HD21	1.99	0.44
1:A:151:LEU:O	1:A:209:LYS:HD2	2.17	0.44
1:E:12:LEU:HD12	1:E:12:LEU:C	2.43	0.44
1:E:152:LYS:NZ	2:F:159:SER:OG	2.50	0.43
3:G:208:ARG:HG3	3:G:208:ARG:HH11	1.82	0.43
1:C:75:SER:O	1:C:76:ALA:HB3	2.18	0.43
2:B:182:LYS:HE2	2:B:210:GLN:OE1	2.18	0.43
1:E:144:PHE:CE1	2:F:164:ALA:O	2.71	0.43
2:F:156:LYS:HE3	2:F:214:LEU:HD21	1.99	0.43
2:F:199:THR:HG23	2:F:200:SER:N	2.32	0.43
1:A:114:GLN:HE21	1:A:122:VAL:HG13	1.84	0.43
1:E:216:LYS:NZ	1:E:237:ARG:HB3	2.33	0.43
1:C:171:LYS:CG	1:C:171:LYS:CE	2.94	0.43
2:D:210:GLN:HG3	2:D:214:LEU:O	2.19	0.43
2:F:184:TYR:CE2	2:F:215:TYR:HB2	2.54	0.43
3:H:219:PRO:O	3:H:220:ALA:C	2.61	0.43
3:G:265:SER:O	3:G:271:LEU:HA	2.19	0.43
1:C:201:LEU:HD23	1:C:201:LEU:C	2.44	0.42
1:E:212:TYR:HA	1:E:218:TYR:OH	2.19	0.42
2:F:199:THR:CG2	2:F:200:SER:N	2.83	0.42
3:I:300:MET:HE2	3:I:300:MET:HB3	1.97	0.42
2:D:109:MET:CE	2:D:148:VAL:HG21	2.47	0.42
1:E:149:SER:CB	2:F:161:PHE:CD1	3.02	0.42
1:A:150:GLN:HG2	1:A:155:THR:O	2.19	0.42
2:B:113:ARG:HG2	2:B:116:ASP:OD2	2.19	0.42
2:B:156:LYS:CG	2:B:157:GLY:N	2.81	0.42
1:E:62:GLN:HB2	1:E:72:LEU:HD11	2.01	0.42
1:E:176:VAL:CG2	1:E:181:GLN:CD	2.92	0.42
1:C:57:ALA:HB1	1:C:116:SER:OG	2.19	0.42
1:E:229:SER:O	1:E:230:PRO:C	2.62	0.42
1:C:52:GLN:NE2	4:C:301:HOH:O	2.28	0.42
2:B:240:LYS:N	2:B:241:PRO:HD2	2.34	0.42
2:F:6:GLN:HB2	2:F:51:SER:OG	2.20	0.42
2:F:109:MET:HE1	2:F:148:VAL:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:223:THR:HG23	4:C:313:HOH:O	2.19	0.42
1:E:176:VAL:HG23	1:E:181:GLN:CD	2.44	0.42
1:C:136:VAL:O	1:A:49:ARG:NH2	2.53	0.41
2:B:158:PRO:HD2	2:B:244:THR:HG21	2.02	0.41
3:G:223:LEU:C	3:G:223:LEU:HD23	2.45	0.41
2:B:6:GLN:HB2	2:B:51:SER:OG	2.20	0.41
1:E:148:ASP:C	1:E:150:GLN:N	2.78	0.41
2:B:213:GLY:C	2:B:214:LEU:HD12	2.45	0.41
1:A:171:LYS:HB3	1:A:223:THR:HB	2.02	0.41
3:G:258:ILE:O	3:G:258:ILE:CG2	2.68	0.41
1:C:193:ASP:HB3	1:C:196:ASP:OD1	2.21	0.41
1:C:233:LYS:HA	1:C:233:LYS:HD3	1.84	0.41
1:A:212:TYR:HA	1:A:218:TYR:OH	2.21	0.41
2:B:77:ILE:HD12	2:B:97:SER:HA	2.03	0.41
1:E:177:ASP:HA	1:E:217:VAL:HG22	2.03	0.41
1:E:213:GLU:HA	1:E:237:ARG:HH11	1.85	0.41
1:C:180:LEU:CD2	1:C:181:GLN:O	2.69	0.40
1:A:145:PRO:HB3	1:A:235:PHE:CZ	2.56	0.40
1:E:13:SER:HA	1:E:131:GLU:O	2.21	0.40
2:D:217:LEU:HD12	2:D:217:LEU:C	2.46	0.40
1:A:53:SER:HA	1:A:94:THR:HG22	2.03	0.40
2:B:5:VAL:HB	2:B:141:TYR:CE2	2.56	0.40
1:A:216:LYS:O	1:A:236:ASN:HA	2.22	0.40
2:B:77:ILE:HG13	2:B:84:THR:HG22	2.03	0.40
1:E:144:PHE:HE1	2:F:164:ALA:O	2.05	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:437:HOH:O	4:H:437:HOH:O[2_553]	1.87	0.33

## 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	211/239 (88%)	207 (98%)	4 (2%)	0	100	100
1	C	210/239 (88%)	205 (98%)	5 (2%)	0	100	100
1	E	211/239 (88%)	201 (95%)	9 (4%)	1 (0%)	25	44
2	B	216/260 (83%)	209 (97%)	7 (3%)	0	100	100
2	D	217/260 (84%)	211 (97%)	6 (3%)	0	100	100
2	F	217/260 (84%)	205 (94%)	12 (6%)	0	100	100
3	G	120/134 (90%)	120 (100%)	0	0	100	100
3	H	125/134 (93%)	120 (96%)	5 (4%)	0	100	100
3	I	121/134 (90%)	121 (100%)	0	0	100	100
All	All	1648/1899 (87%)	1599 (97%)	48 (3%)	1 (0%)	48	69

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	153	SER

### 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	187/208 (90%)	186 (100%)	1 (0%)	86	95
1	C	187/208 (90%)	181 (97%)	6 (3%)	34	60
1	E	187/208 (90%)	181 (97%)	6 (3%)	34	60
2	B	184/218 (84%)	177 (96%)	7 (4%)	28	53
2	D	185/218 (85%)	182 (98%)	3 (2%)	58	80
2	F	181/218 (83%)	177 (98%)	4 (2%)	47	73
3	G	106/118 (90%)	105 (99%)	1 (1%)	75	90
3	H	111/118 (94%)	109 (98%)	2 (2%)	54	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	I	107/118 (91%)	103 (96%)	4 (4%)	29 55
All	All	1435/1632 (88%)	1401 (98%)	34 (2%)	44 70

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	13	SER
1	C	39	SER
1	C	73	ILE
1	C	148	ASP
1	C	171	LYS
1	C	221	GLU
2	D	152	SER
2	D	199	THR
2	D	217	LEU
1	A	188	SER
2	B	10	SER
2	B	69	LYS
2	B	111	SER
2	B	152	SER
2	B	188	PRO
2	B	226	SER
2	B	232	THR
1	E	143	ILE
1	E	151	LEU
1	E	158	VAL
1	E	180	LEU
1	E	206	THR
1	E	216	LYS
2	F	43	SER
2	F	159	SER
2	F	166	SER
2	F	235	CYS
3	G	263	ILE
3	I	229	SER
3	I	237	LYS
3	I	242	LEU
3	I	283	LYS
3	H	206	THR
3	H	237	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23)

such sidechains are listed below:

Mol	Chain	Res	Type
1	C	4	GLN
1	C	173	GLN
1	C	215	HIS
2	D	210	GLN
2	D	238	ASN
1	A	163	ASN
1	A	192	GLN
2	B	103	ASN
2	B	203	HIS
1	E	4	GLN
1	E	63	GLN
1	E	104	GLN
1	E	178	ASN
2	F	65	GLN
2	F	103	ASN
2	F	133	HIS
2	F	144	GLN
2	F	203	HIS
3	G	269	ASN
3	G	309	ASN
3	I	249	GLN
3	H	295	GLN
3	H	309	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	213/239 (89%)	-0.46	1 (0%) 87 85	34, 52, 95, 121	0
1	C	212/239 (88%)	-0.39	1 (0%) 87 85	33, 52, 98, 108	0
1	E	213/239 (89%)	0.02	16 (7%) 22 20	33, 52, 128, 142	0
2	B	220/260 (84%)	-0.16	4 (1%) 67 64	35, 67, 106, 121	0
2	D	221/260 (85%)	-0.22	5 (2%) 61 58	33, 55, 110, 134	0
2	F	221/260 (85%)	0.03	16 (7%) 23 21	32, 58, 125, 145	0
3	G	122/134 (91%)	-0.65	1 (0%) 82 79	33, 46, 66, 81	0
3	H	126/134 (94%)	-0.49	3 (2%) 59 56	27, 49, 77, 115	1 (0%)
3	I	123/134 (91%)	-0.53	1 (0%) 82 79	38, 49, 73, 98	0
All	All	1671/1899 (87%)	-0.27	48 (2%) 54 50	27, 53, 111, 145	1 (0%)

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	210	ALA	5.2
1	E	1	SER	4.7
1	E	153	SER	4.2
2	F	252	PRO	4.2
1	E	218	TYR	3.6
1	E	151	LEU	3.6
3	I	199	ILE	3.5
2	B	252	PRO	3.4
2	F	173	GLY	3.4
1	E	154	GLY	3.3
2	F	230	THR	3.3
2	F	167	SER	3.2
2	F	166	SER	3.2
1	E	150	GLN	3.2
2	F	228	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	1	SER	3.1
2	F	162	PRO	3.1
1	E	155	THR	3.0
2	D	252	PRO	2.9
1	E	217	VAL	2.9
3	H	322	VAL	2.8
2	D	228	LEU	2.8
2	F	251	GLU	2.8
1	E	149	SER	2.7
1	E	209	LYS	2.6
2	D	227	SER	2.6
3	H	199	ILE	2.6
2	F	161	PHE	2.6
1	E	207	LEU	2.6
3	G	322	VAL	2.5
1	E	148	ASP	2.5
3	H	197	LYS	2.4
2	B	166	SER	2.4
2	F	227	SER	2.3
2	F	178	GLY	2.3
2	B	69	LYS	2.3
2	F	199	THR	2.2
1	E	180	LEU	2.2
2	F	248	LYS	2.2
2	D	167	SER	2.2
1	E	158	VAL	2.2
2	F	163	LEU	2.1
2	D	173	GLY	2.1
1	C	171	LYS	2.1
1	E	144	PHE	2.0
2	B	232	THR	2.0
2	F	249	LYS	2.0
2	F	232	THR	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.