



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:24 AM UTC

PDB ID : 4KWB / pdb_00004kwb
Title : Structure of signal peptide peptidase A with C-termini bound in the active sites: insights into specificity, self-processing and regulation
Authors : Nam, S.E.; Paetzel, M.
Deposited on : 2013-05-23
Resolution : 2.39 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

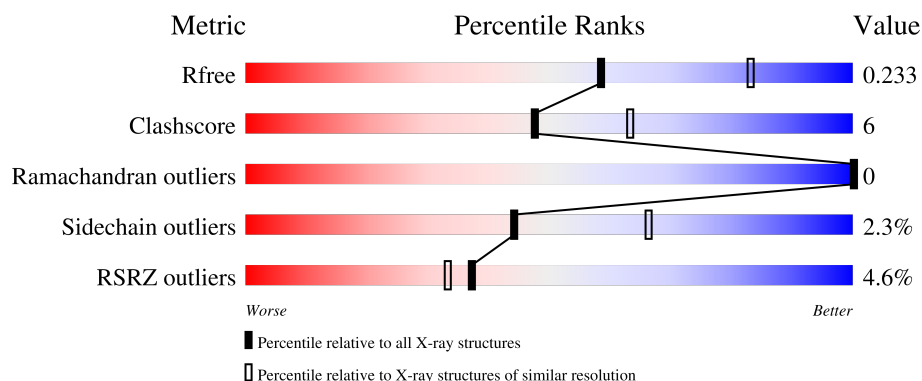
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	273	0% 79% 7% 13%
1	B	273	3% 78% 7% 15%
1	C	273	3% 75% 10% 13%
1	D	273	7% 71% 11% 16%
1	E	273	5% 73% 11% 15%

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Mol	Chain	Length	Quality of chain
1	F	273	
1	G	273	
1	H	273	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14324 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 Signal peptide peptidase SppA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	0	0
			1797	1133	297	356	11			
1	B	233	Total	C	N	O	S	0	0	0
			1754	1103	292	348	11			
1	C	237	Total	C	N	O	S	0	0	0
			1808	1138	300	359	11			
1	D	228	Total	C	N	O	S	0	0	0
			1686	1063	280	332	11			
1	E	232	Total	C	N	O	S	0	0	0
			1747	1097	293	346	11			
1	F	234	Total	C	N	O	S	0	0	0
			1779	1122	294	352	11			
1	G	232	Total	C	N	O	S	0	0	0
			1756	1102	294	349	11			
1	H	232	Total	C	N	O	S	0	0	0
			1776	1119	297	349	11			

There are 104 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	199	ALA	LYS	engineered mutation	UNP O34525
A	?	-	LEU	SEE REMARK 999	UNP O34525
A	?	-	GLY	SEE REMARK 999	UNP O34525
A	?	-	SER	SEE REMARK 999	UNP O34525
A	?	-	LEU	SEE REMARK 999	UNP O34525
A	?	-	PHE	SEE REMARK 999	UNP O34525
A	?	-	SER	SEE REMARK 999	UNP O34525
A	?	-	MET	SEE REMARK 999	UNP O34525
A	?	-	GLY	SEE REMARK 999	UNP O34525
A	?	-	ALA	SEE REMARK 999	UNP O34525
A	?	-	ASN	SEE REMARK 999	UNP O34525
A	?	-	LYS	SEE REMARK 999	UNP O34525
A	?	-	MET	SEE REMARK 999	UNP O34525

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Chain	Residue	Modelled	Actual	Comment	Reference
B	199	ALA	LYS	engineered mutation	UNP O34525
B	?	-	LEU	SEE REMARK 999	UNP O34525
B	?	-	GLY	SEE REMARK 999	UNP O34525
B	?	-	SER	SEE REMARK 999	UNP O34525
B	?	-	LEU	SEE REMARK 999	UNP O34525
B	?	-	PHE	SEE REMARK 999	UNP O34525
B	?	-	SER	SEE REMARK 999	UNP O34525
B	?	-	MET	SEE REMARK 999	UNP O34525
B	?	-	GLY	SEE REMARK 999	UNP O34525
B	?	-	ALA	SEE REMARK 999	UNP O34525
B	?	-	ASN	SEE REMARK 999	UNP O34525
B	?	-	LYS	SEE REMARK 999	UNP O34525
B	?	-	MET	SEE REMARK 999	UNP O34525
C	199	ALA	LYS	engineered mutation	UNP O34525
C	?	-	LEU	SEE REMARK 999	UNP O34525
C	?	-	GLY	SEE REMARK 999	UNP O34525
C	?	-	SER	SEE REMARK 999	UNP O34525
C	?	-	LEU	SEE REMARK 999	UNP O34525
C	?	-	PHE	SEE REMARK 999	UNP O34525
C	?	-	SER	SEE REMARK 999	UNP O34525
C	?	-	MET	SEE REMARK 999	UNP O34525
C	?	-	GLY	SEE REMARK 999	UNP O34525
C	?	-	ALA	SEE REMARK 999	UNP O34525
C	?	-	ASN	SEE REMARK 999	UNP O34525
C	?	-	LYS	SEE REMARK 999	UNP O34525
C	?	-	MET	SEE REMARK 999	UNP O34525
D	199	ALA	LYS	engineered mutation	UNP O34525
D	?	-	LEU	SEE REMARK 999	UNP O34525
D	?	-	GLY	SEE REMARK 999	UNP O34525
D	?	-	SER	SEE REMARK 999	UNP O34525
D	?	-	LEU	SEE REMARK 999	UNP O34525
D	?	-	PHE	SEE REMARK 999	UNP O34525
D	?	-	SER	SEE REMARK 999	UNP O34525
D	?	-	MET	SEE REMARK 999	UNP O34525
D	?	-	GLY	SEE REMARK 999	UNP O34525
D	?	-	ALA	SEE REMARK 999	UNP O34525
D	?	-	ASN	SEE REMARK 999	UNP O34525
D	?	-	LYS	SEE REMARK 999	UNP O34525
D	?	-	MET	SEE REMARK 999	UNP O34525
E	199	ALA	LYS	engineered mutation	UNP O34525
E	?	-	LEU	SEE REMARK 999	UNP O34525
E	?	-	GLY	SEE REMARK 999	UNP O34525

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Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	SER	SEE REMARK 999	UNP O34525
E	?	-	LEU	SEE REMARK 999	UNP O34525
E	?	-	PHE	SEE REMARK 999	UNP O34525
E	?	-	SER	SEE REMARK 999	UNP O34525
E	?	-	MET	SEE REMARK 999	UNP O34525
E	?	-	GLY	SEE REMARK 999	UNP O34525
E	?	-	ALA	SEE REMARK 999	UNP O34525
E	?	-	ASN	SEE REMARK 999	UNP O34525
E	?	-	LYS	SEE REMARK 999	UNP O34525
E	?	-	MET	SEE REMARK 999	UNP O34525
F	199	ALA	LYS	engineered mutation	UNP O34525
F	?	-	LEU	SEE REMARK 999	UNP O34525
F	?	-	GLY	SEE REMARK 999	UNP O34525
F	?	-	SER	SEE REMARK 999	UNP O34525
F	?	-	LEU	SEE REMARK 999	UNP O34525
F	?	-	PHE	SEE REMARK 999	UNP O34525
F	?	-	SER	SEE REMARK 999	UNP O34525
F	?	-	MET	SEE REMARK 999	UNP O34525
F	?	-	GLY	SEE REMARK 999	UNP O34525
F	?	-	ALA	SEE REMARK 999	UNP O34525
F	?	-	ASN	SEE REMARK 999	UNP O34525
F	?	-	LYS	SEE REMARK 999	UNP O34525
F	?	-	MET	SEE REMARK 999	UNP O34525
G	199	ALA	LYS	engineered mutation	UNP O34525
G	?	-	LEU	SEE REMARK 999	UNP O34525
G	?	-	GLY	SEE REMARK 999	UNP O34525
G	?	-	SER	SEE REMARK 999	UNP O34525
G	?	-	LEU	SEE REMARK 999	UNP O34525
G	?	-	PHE	SEE REMARK 999	UNP O34525
G	?	-	SER	SEE REMARK 999	UNP O34525
G	?	-	MET	SEE REMARK 999	UNP O34525
G	?	-	GLY	SEE REMARK 999	UNP O34525
G	?	-	ALA	SEE REMARK 999	UNP O34525
G	?	-	ASN	SEE REMARK 999	UNP O34525
G	?	-	LYS	SEE REMARK 999	UNP O34525
G	?	-	MET	SEE REMARK 999	UNP O34525
H	199	ALA	LYS	engineered mutation	UNP O34525
H	?	-	LEU	SEE REMARK 999	UNP O34525
H	?	-	GLY	SEE REMARK 999	UNP O34525
H	?	-	SER	SEE REMARK 999	UNP O34525
H	?	-	LEU	SEE REMARK 999	UNP O34525
H	?	-	PHE	SEE REMARK 999	UNP O34525

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Chain	Residue	Modelled	Actual	Comment	Reference
H	?	-	SER	SEE REMARK 999	UNP O34525
H	?	-	MET	SEE REMARK 999	UNP O34525
H	?	-	GLY	SEE REMARK 999	UNP O34525
H	?	-	ALA	SEE REMARK 999	UNP O34525
H	?	-	ASN	SEE REMARK 999	UNP O34525
H	?	-	LYS	SEE REMARK 999	UNP O34525
H	?	-	MET	SEE REMARK 999	UNP O34525

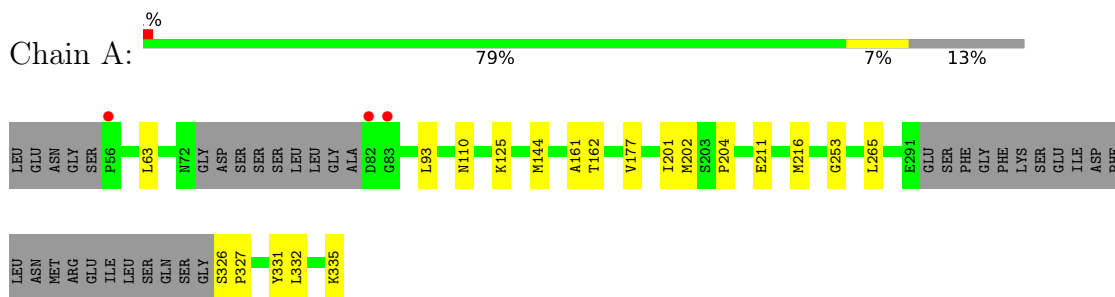
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	36	Total O 36 36	0	0
2	B	22	Total O 22 22	0	0
2	C	31	Total O 31 31	0	0
2	D	19	Total O 19 19	0	0
2	E	21	Total O 21 21	0	0
2	F	35	Total O 35 35	0	0
2	G	24	Total O 24 24	0	0
2	H	33	Total O 33 33	0	0

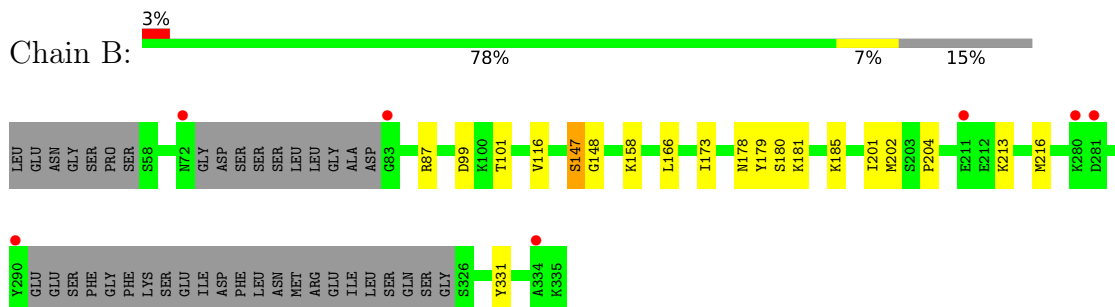
3 Residue-property plots [i](#)

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.

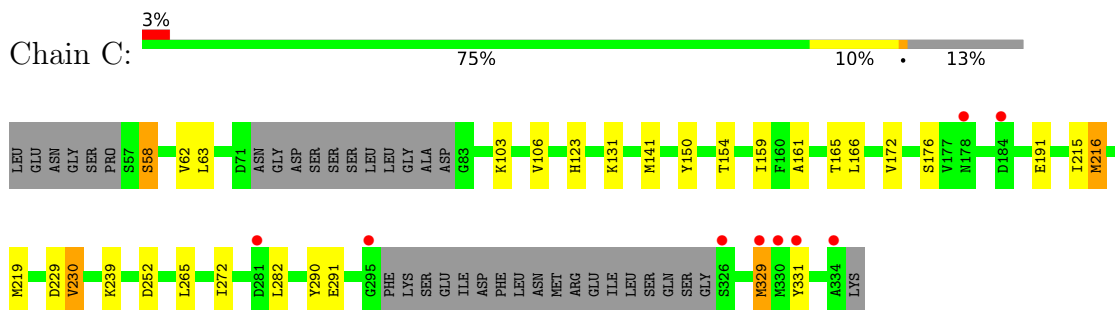
- Molecule 1: Signal peptide peptidase SppA



- Molecule 1: Signal peptide peptidase SppA

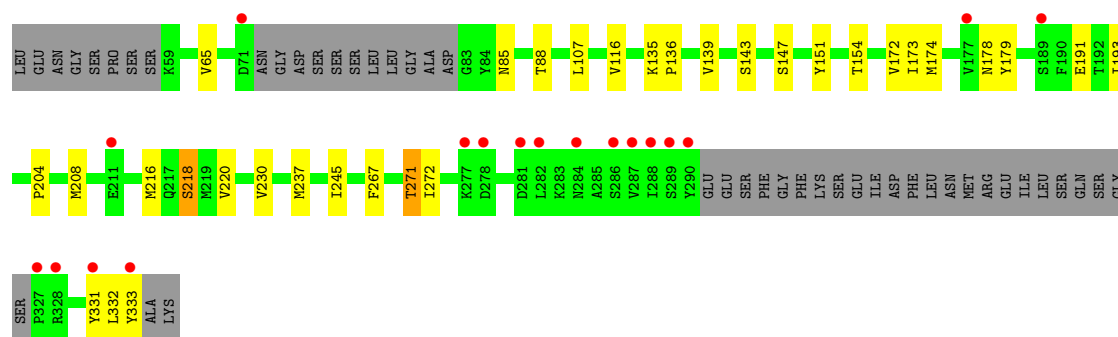


- Molecule 1: Signal peptide peptidase SppA

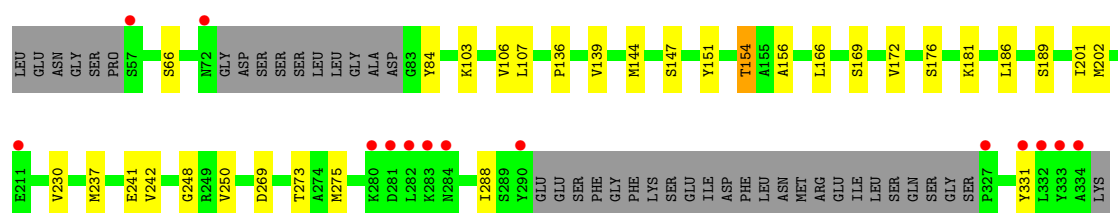
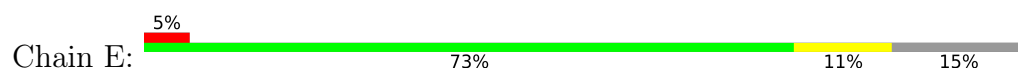


- Molecule 1: Signal peptide peptidase SppA

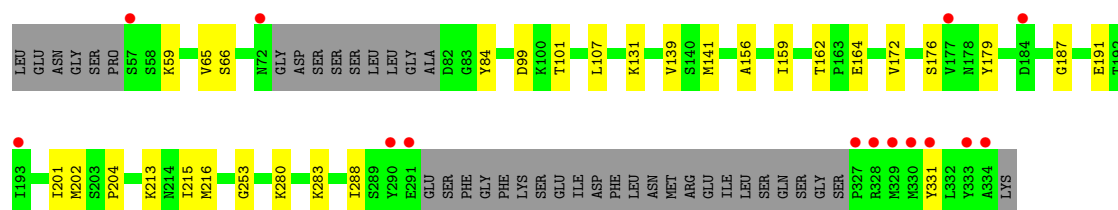
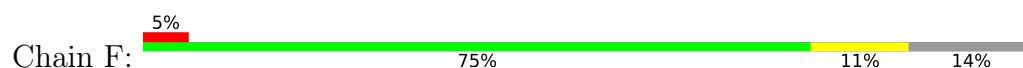




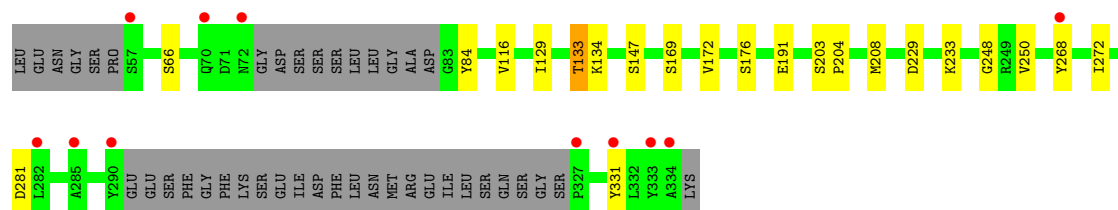
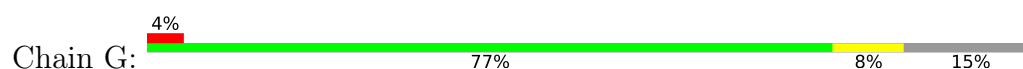
- Molecule 1: Signal peptide peptidase SppA



- Molecule 1: Signal peptide peptidase SppA

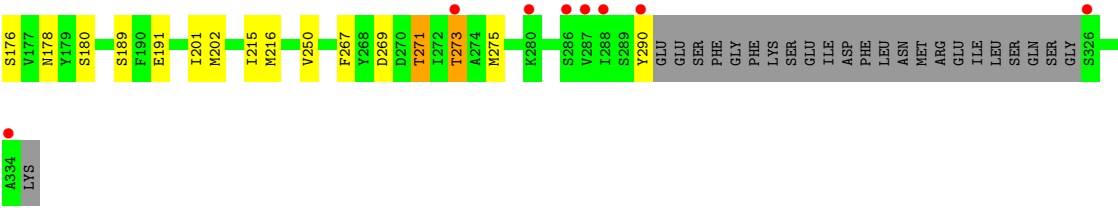


- Molecule 1: Signal peptide peptidase SppA



- Molecule 1: Signal peptide peptidase SppA





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	87.80Å 130.98Å 207.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.39 50.00 – 2.39	Depositor EDS
% Data completeness (in resolution range)	98.7 (50.00-2.39) 98.7 (50.00-2.39)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.13 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.206 , 0.240 0.203 , 0.233	Depositor DCC
R_{free} test set	4716 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	45.7	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 46.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14324	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.58	0/1821	0.80	0/2441
1	B	0.61	0/1778	0.76	0/2390
1	C	0.58	0/1833	0.81	0/2458
1	D	0.54	0/1708	0.82	0/2298
1	E	0.57	0/1769	0.80	0/2374
1	F	0.56	0/1803	0.81	0/2417
1	G	0.53	0/1778	0.77	0/2386
1	H	0.54	0/1800	0.79	0/2413
All	All	0.56	0/14290	0.80	0/19177

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1797	0	1786	16	0
1	B	1754	0	1721	19	0
1	C	1808	0	1799	35	0
1	D	1686	0	1629	28	0
1	E	1747	0	1727	26	0
1	F	1779	0	1781	25	0
1	G	1756	0	1742	17	0
1	H	1776	0	1784	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	36	0	0	0	0
2	B	22	0	0	0	0
2	C	31	0	0	0	0
2	D	19	0	0	1	0
2	E	21	0	0	0	0
2	F	35	0	0	0	0
2	G	24	0	0	0	0
2	H	33	0	0	1	0
All	All	14324	0	13969	156	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 6.

All (156) 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:D:333:TYR:HD2	1:E:144:MET:HE1	1.27	0.95
1:H:215:ILE:HG22	1:H:216:MET:HE2	1.49	0.95
1:A:326:SER:HB2	1:A:327:PRO:HD3	1.52	0.89
1:D:333:TYR:CD2	1:E:144:MET:HE1	2.06	0.89
1:D:218:SER:HB3	2:D:409:HOH:O	1.71	0.88
1:C:329:MET:H	1:C:329:MET:HE3	1.44	0.82
1:E:106:VAL:HG23	1:E:275:MET:HE2	1.64	0.79
1:F:215:ILE:HG22	1:F:216:MET:HE2	1.66	0.78
1:A:201:ILE:CD1	1:A:216:MET:HE2	2.15	0.77
1:F:201:ILE:CD1	1:F:216:MET:HE3	2.15	0.75
1:E:176:SER:OG	1:F:191:GLU:HB3	1.87	0.74
1:B:213:LYS:HE2	1:C:191:GLU:OE1	1.87	0.73
1:C:216:MET:HA	1:C:216:MET:HE2	1.72	0.71
1:A:202:MET:HG2	1:A:216:MET:HE3	1.72	0.71
1:F:59:LYS:HD3	1:F:288:ILE:HG12	1.73	0.71
1:F:176:SER:OG	1:G:191:GLU:HB3	1.91	0.71
1:F:201:ILE:HD13	1:F:216:MET:HE3	1.73	0.70
1:C:62:VAL:HG22	1:C:106:VAL:CG1	2.22	0.70
1:H:201:ILE:CD1	1:H:216:MET:HE3	2.24	0.68
1:H:201:ILE:HD13	1:H:216:MET:HE3	1.76	0.68
1:G:176:SER:OG	1:H:191:GLU:HB3	1.93	0.68
1:A:201:ILE:HD13	1:A:216:MET:HE2	1.76	0.67
1:C:215:ILE:HG22	1:C:216:MET:CE	2.26	0.66
1:D:333:TYR:CD2	1:E:144:MET:CE	2.79	0.66
1:C:106:VAL:HG11	1:C:272:ILE:HD11	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:151:TYR:O	1:D:154:THR:HG22	1.96	0.65
1:F:99:ASP:OD1	1:F:101:THR:HG22	1.97	0.64
1:B:179:TYR:CE2	1:B:204:PRO:HB2	2.33	0.64
1:G:250:VAL:CG2	1:H:216:MET:HE1	2.28	0.62
1:C:216:MET:HB3	1:D:193:ILE:HD13	1.82	0.61
1:C:154:THR:OG1	1:C:230:VAL:HG13	2.01	0.61
1:D:331:TYR:CE1	1:E:172:VAL:HG22	2.35	0.61
1:F:65:VAL:HG23	1:F:107:LEU:HD11	1.82	0.61
1:C:62:VAL:HG22	1:C:106:VAL:HG13	1.82	0.60
1:E:237:MET:HE2	1:E:242:VAL:HG22	1.83	0.60
1:B:99:ASP:OD1	1:B:101:THR:HG22	2.02	0.60
1:D:174:MET:HE3	1:D:216:MET:HE3	1.83	0.60
1:E:331:TYR:CE1	1:F:172:VAL:HG22	2.37	0.59
1:D:65:VAL:HG23	1:D:107:LEU:HD11	1.84	0.59
1:G:129:ILE:O	1:G:133:THR:HG22	2.03	0.59
1:C:216:MET:CE	1:C:216:MET:CA	2.80	0.59
1:C:329:MET:H	1:C:329:MET:CE	2.13	0.58
1:D:331:TYR:HE1	1:E:172:VAL:HG22	1.67	0.58
1:E:237:MET:HE3	1:E:241:GLU:HG2	1.83	0.58
1:C:216:MET:HE2	1:C:216:MET:CA	2.34	0.57
1:B:213:LYS:CE	1:C:191:GLU:OE1	2.52	0.57
1:D:107:LEU:HB3	1:D:139:VAL:HG12	1.85	0.57
1:E:144:MET:HE3	1:E:166:LEU:HD22	1.86	0.56
1:H:269:ASP:O	1:H:273:THR:HG23	2.06	0.56
1:F:331:TYR:CE1	1:G:172:VAL:HG22	2.41	0.56
1:C:216:MET:N	1:C:216:MET:HE3	2.21	0.55
1:B:201:ILE:CD1	1:B:216:MET:HE2	2.37	0.55
1:H:130:LYS:HG2	2:H:414:HOH:O	2.05	0.55
1:H:267:PHE:O	1:H:271:THR:HG23	2.07	0.55
1:F:201:ILE:HD11	1:F:216:MET:HE3	1.87	0.55
1:B:178:ASN:OD1	1:B:180:SER:HB3	2.06	0.54
1:D:174:MET:HE2	1:D:220:VAL:HG23	1.90	0.54
1:H:178:ASN:HD22	1:H:180:SER:H	1.55	0.54
1:A:326:SER:HB2	1:A:327:PRO:CD	2.31	0.53
1:B:331:TYR:CE1	1:C:172:VAL:HG22	2.44	0.53
1:B:201:ILE:HD13	1:B:216:MET:HE2	1.90	0.52
1:A:332:LEU:HD23	1:A:335:LYS:HD2	1.92	0.52
1:G:268:TYR:CZ	1:G:272:ILE:HD11	2.45	0.52
1:C:166:LEU:HB2	1:C:329:MET:HE1	1.90	0.52
1:B:201:ILE:HD13	1:B:216:MET:CE	2.40	0.51
1:H:176:SER:HB2	1:H:202:MET:HE1	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:VAL:HG11	1:C:272:ILE:CD1	2.40	0.51
1:C:331:TYR:CE1	1:D:172:VAL:HG22	2.45	0.51
1:C:331:TYR:CD2	1:D:116:VAL:HA	2.47	0.50
1:E:331:TYR:HE1	1:F:172:VAL:HG22	1.75	0.50
1:G:250:VAL:HG22	1:H:216:MET:HE1	1.93	0.50
1:C:215:ILE:HG22	1:C:216:MET:HE1	1.93	0.50
1:D:174:MET:CE	1:D:216:MET:HE3	2.42	0.50
1:F:139:VAL:HG23	1:F:156:ALA:HB2	1.95	0.49
1:F:164:GLU:HB3	1:G:116:VAL:HG23	1.95	0.49
1:E:269:ASP:O	1:E:273:THR:HG23	2.13	0.49
1:D:267:PHE:O	1:D:271:THR:HG23	2.12	0.48
1:C:58:SER:HB3	1:C:103:LYS:HD2	1.95	0.48
1:G:66:SER:O	1:G:84:TYR:HB2	2.13	0.48
1:C:331:TYR:HE1	1:D:172:VAL:HG22	1.78	0.48
1:F:66:SER:O	1:F:84:TYR:HB2	2.13	0.48
1:C:216:MET:CE	1:C:216:MET:N	2.77	0.48
1:H:63:LEU:HD21	1:H:290:TYR:HD2	1.77	0.48
1:H:201:ILE:HD11	1:H:216:MET:HE3	1.96	0.48
1:D:178:ASN:ND2	1:E:189:SER:HB3	2.29	0.48
1:E:154:THR:HG21	1:E:230:VAL:HB	1.95	0.48
1:H:169:SER:HB2	1:H:250:VAL:HG12	1.96	0.47
1:A:177:VAL:O	1:A:204:PRO:HA	2.14	0.47
1:G:331:TYR:CE1	1:H:172:VAL:HG22	2.49	0.47
1:E:107:LEU:HB3	1:E:139:VAL:HG22	1.97	0.47
1:E:103:LYS:O	1:E:136:PRO:HD2	2.14	0.47
1:F:162:THR:O	1:F:253:GLY:HA3	2.15	0.47
1:F:331:TYR:HE1	1:G:172:VAL:HG22	1.81	0.46
1:C:141:MET:HE1	1:C:150:TYR:HD2	1.81	0.46
1:C:229:ASP:OD1	1:C:239:LYS:NZ	2.41	0.46
1:F:179:TYR:CE2	1:F:204:PRO:HB2	2.51	0.46
1:D:331:TYR:C	1:E:147:SER:OG	2.58	0.46
1:A:161:ALA:O	1:A:265:LEU:HA	2.15	0.46
1:C:123:HIS:CE1	1:C:230:VAL:HG22	2.51	0.45
1:H:215:ILE:HG22	1:H:216:MET:CE	2.32	0.45
1:A:331:TYR:CD2	1:B:116:VAL:HA	2.51	0.45
1:D:237:MET:HE1	1:D:245:ILE:HD12	1.97	0.45
1:G:169:SER:HA	1:G:248:GLY:O	2.15	0.45
1:E:169:SER:HA	1:E:248:GLY:O	2.17	0.45
1:H:136:PRO:HB2	1:H:275:MET:HE2	1.98	0.45
1:D:85:ASN:HB3	1:D:88:THR:HB	1.99	0.44
1:C:176:SER:HB3	1:D:191:GLU:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:208:MET:HE1	1:D:216:MET:HG3	1.98	0.44
1:E:151:TYR:O	1:E:154:THR:HB	2.18	0.44
1:A:162:THR:O	1:A:253:GLY:HA3	2.17	0.44
1:C:63:LEU:HD21	1:C:290:TYR:HD2	1.83	0.44
1:D:179:TYR:CE2	1:D:204:PRO:HB2	2.52	0.44
1:C:216:MET:HA	1:C:216:MET:CE	2.42	0.44
1:C:161:ALA:O	1:C:265:LEU:HA	2.18	0.44
1:H:59:LYS:N	1:H:101:THR:O	2.51	0.44
1:C:165:THR:O	1:C:252:ASP:HA	2.18	0.44
1:H:110:ASN:HA	1:H:144:MET:O	2.18	0.43
1:H:160:PHE:CG	1:H:271:THR:HG22	2.53	0.43
1:E:250:VAL:HG22	1:F:216:MET:HE1	2.00	0.43
1:H:166:LEU:C	1:H:166:LEU:HD23	2.43	0.43
1:H:174:MET:HE3	1:H:174:MET:HB3	1.93	0.43
1:F:141:MET:HE3	1:F:159:ILE:HG21	2.00	0.43
1:H:141:MET:HE3	1:H:159:ILE:HG21	2.00	0.43
1:A:331:TYR:O	1:B:147:SER:HB3	2.19	0.43
1:A:202:MET:CG	1:A:216:MET:HE3	2.47	0.42
1:B:166:LEU:HG	1:C:219:MET:HE1	2.01	0.42
1:H:64:GLU:HG2	1:H:108:LYS:HB2	2.01	0.42
1:A:63:LEU:HD13	1:A:93:LEU:HD13	2.01	0.42
1:B:201:ILE:O	1:B:202:MET:HB2	2.20	0.42
1:B:213:LYS:NZ	1:C:191:GLU:OE1	2.52	0.42
1:E:66:SER:O	1:E:84:TYR:HB2	2.20	0.42
1:B:213:LYS:HE2	1:C:191:GLU:CD	2.45	0.42
1:G:229:ASP:OD1	1:G:233:LYS:NZ	2.48	0.42
1:F:176:SER:HB3	1:F:202:MET:HE1	2.00	0.42
1:G:208:MET:HE3	1:G:208:MET:HB2	1.94	0.42
1:E:201:ILE:O	1:E:202:MET:HB2	2.19	0.42
1:D:267:PHE:O	1:D:271:THR:CG2	2.67	0.41
1:D:178:ASN:HD21	1:E:189:SER:HB3	1.85	0.41
1:A:201:ILE:HG12	1:A:216:MET:CE	2.51	0.41
1:C:141:MET:HE3	1:C:159:ILE:HG21	2.02	0.41
1:F:213:LYS:HD3	1:G:191:GLU:OE2	2.21	0.41
1:A:110:ASN:HA	1:A:144:MET:O	2.21	0.41
1:G:331:TYR:CD2	1:H:116:VAL:HA	2.56	0.41
1:F:280:LYS:O	1:F:283:LYS:HB2	2.21	0.41
1:H:139:VAL:HG23	1:H:156:ALA:HB2	2.02	0.41
1:B:201:ILE:CD1	1:B:216:MET:CE	2.97	0.41
1:A:125:LYS:HD3	1:A:125:LYS:HA	1.97	0.41
1:B:166:LEU:C	1:B:166:LEU:HD23	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:ARG:HD3	1:B:87:ARG:HA	1.84	0.41
1:D:135:LYS:HA	1:D:136:PRO:HD3	1.96	0.41
1:E:139:VAL:HG23	1:E:156:ALA:HB2	2.02	0.41
1:B:147:SER:HB3	1:B:148:GLY:H	1.66	0.40
1:E:181:LYS:HB2	1:F:187:GLY:HA3	2.04	0.40
1:D:154:THR:HG21	1:D:230:VAL:HB	2.04	0.40
1:F:201:ILE:HD13	1:F:216:MET:CE	2.47	0.40
1:G:203:SER:HA	1:G:204:PRO:HD3	1.95	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	231/273 (85%)	227 (98%)	4 (2%)	0	100	100
1	B	227/273 (83%)	220 (97%)	7 (3%)	0	100	100
1	C	231/273 (85%)	228 (99%)	3 (1%)	0	100	100
1	D	222/273 (81%)	216 (97%)	6 (3%)	0	100	100
1	E	226/273 (83%)	220 (97%)	6 (3%)	0	100	100
1	F	228/273 (84%)	225 (99%)	3 (1%)	0	100	100
1	G	226/273 (83%)	219 (97%)	7 (3%)	0	100	100
1	H	226/273 (83%)	220 (97%)	6 (3%)	0	100	100
All	All	1817/2184 (83%)	1775 (98%)	42 (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	190/231 (82%)	189 (100%)	1 (0%)	81	91
1	B	184/231 (80%)	179 (97%)	5 (3%)	39	62
1	C	194/231 (84%)	187 (96%)	7 (4%)	31	52
1	D	170/231 (74%)	163 (96%)	7 (4%)	27	46
1	E	184/231 (80%)	181 (98%)	3 (2%)	55	76
1	F	191/231 (83%)	190 (100%)	1 (0%)	81	91
1	G	187/231 (81%)	183 (98%)	4 (2%)	47	69
1	H	191/231 (83%)	185 (97%)	6 (3%)	35	57
All	All	1491/1848 (81%)	1457 (98%)	34 (2%)	44	66

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

Mol	Chain	Res	Type
1	A	211	GLU
1	B	147	SER
1	B	158	LYS
1	B	173	ILE
1	B	181	LYS
1	B	185	LYS
1	C	58	SER
1	C	131	LYS
1	C	216	MET
1	C	230	VAL
1	C	282	LEU
1	C	291	GLU
1	C	329	MET
1	D	143	SER
1	D	147	SER
1	D	173	ILE
1	D	218	SER
1	D	271	THR
1	D	272	ILE

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Mol	Chain	Res	Type
1	D	332	LEU
1	E	154	THR
1	E	186	LEU
1	E	288	ILE
1	F	131	LYS
1	G	133	THR
1	G	134	LYS
1	G	147	SER
1	G	281	ASP
1	H	147	SER
1	H	158	LYS
1	H	174	MET
1	H	189	SER
1	H	271	THR
1	H	273	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	178	ASN
1	B	110	ASN
1	B	198	HIS
1	C	70	GLN
1	C	123	HIS
1	C	214	ASN
1	C	217	GLN
1	D	222	ASN
1	E	70	GLN
1	E	110	ASN
1	E	214	ASN
1	E	217	GLN
1	F	110	ASN
1	F	279	HIS
1	G	70	GLN
1	G	110	ASN
1	G	178	ASN
1	G	214	ASN
1	G	222	ASN
1	G	279	HIS
1	H	70	GLN
1	H	178	ASN
1	H	279	HIS

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	237/273 (86%)	-0.08	3 (1%) 75 71	26, 40, 61, 70	0
1	B	233/273 (85%)	0.24	7 (3%) 52 48	33, 50, 92, 106	0
1	C	237/273 (86%)	0.09	9 (3%) 44 40	30, 44, 64, 74	0
1	D	228/273 (83%)	0.55	18 (7%) 18 15	36, 55, 106, 122	0
1	E	232/273 (84%)	0.42	14 (6%) 27 24	32, 52, 101, 122	0
1	F	234/273 (85%)	0.11	14 (5%) 27 24	27, 42, 68, 82	0
1	G	232/273 (84%)	0.27	11 (4%) 36 32	30, 49, 93, 114	0
1	H	232/273 (84%)	0.13	10 (4%) 40 36	30, 46, 74, 90	0
All	All	1865/2184 (85%)	0.21	86 (4%) 37 33	26, 46, 86, 122	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	290	TYR	5.9
1	D	290	TYR	5.1
1	F	334	ALA	5.0
1	G	334	ALA	4.9
1	E	72	ASN	4.8
1	E	327	PRO	4.8
1	D	287	VAL	4.2
1	F	331	TYR	4.2
1	G	72	ASN	4.2
1	A	56	PRO	4.2
1	E	284	ASN	4.1
1	E	290	TYR	4.0
1	E	281	ASP	4.0
1	G	327	PRO	3.9
1	E	333	TYR	3.8
1	E	334	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
1	E	282	LEU	3.8
1	H	290	TYR	3.7
1	F	291	GLU	3.7
1	C	334	ALA	3.6
1	F	333	TYR	3.5
1	G	333	TYR	3.5
1	E	57	SER	3.4
1	H	58	SER	3.4
1	G	57	SER	3.3
1	D	289	SER	3.2
1	C	331	TYR	3.2
1	D	282	LEU	3.2
1	E	331	TYR	3.1
1	B	290	TYR	3.1
1	B	72	ASN	2.9
1	B	211	GLU	2.8
1	F	330	MET	2.8
1	D	281	ASP	2.8
1	D	284	ASN	2.8
1	F	57	SER	2.8
1	D	278	ASP	2.8
1	H	72	ASN	2.8
1	D	327	PRO	2.8
1	D	177	VAL	2.8
1	H	286	SER	2.7
1	D	288	ILE	2.7
1	E	280	LYS	2.7
1	F	327	PRO	2.7
1	H	326	SER	2.7
1	B	280	LYS	2.6
1	C	295	GLY	2.6
1	B	281	ASP	2.6
1	D	328	ARG	2.6
1	B	334	ALA	2.5
1	F	72	ASN	2.5
1	H	334	ALA	2.5
1	F	193	ILE	2.4
1	G	70	GLN	2.4
1	D	277	LYS	2.4
1	H	287	VAL	2.4
1	C	178	ASN	2.3
1	B	83	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	286	SER	2.3
1	F	329	MET	2.3
1	D	189	SER	2.3
1	F	177	VAL	2.3
1	D	331	TYR	2.3
1	F	290	TYR	2.3
1	H	273	THR	2.3
1	E	211	GLU	2.3
1	D	71	ASP	2.2
1	F	184	ASP	2.2
1	A	83	GLY	2.2
1	H	280	LYS	2.2
1	C	330	MET	2.2
1	C	326	SER	2.2
1	G	268	TYR	2.2
1	C	184	ASP	2.2
1	D	211	GLU	2.2
1	G	331	TYR	2.1
1	A	82	ASP	2.1
1	H	288	ILE	2.1
1	F	328	ARG	2.1
1	G	285	ALA	2.1
1	E	283	LYS	2.1
1	C	329	MET	2.1
1	D	333	TYR	2.1
1	C	281	ASP	2.0
1	E	332	LEU	2.0
1	G	282	LEU	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.