



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:05 AM UTC

PDB ID : 3VJB / pdb_00003vjb
Title : Crystal structure of the human squalene synthase
Authors : Liu, C.I.; Jeng, W.Y.; Chang, W.J.; Wang, A.H.J.
Deposited on : 2011-10-14
Resolution : 2.05 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

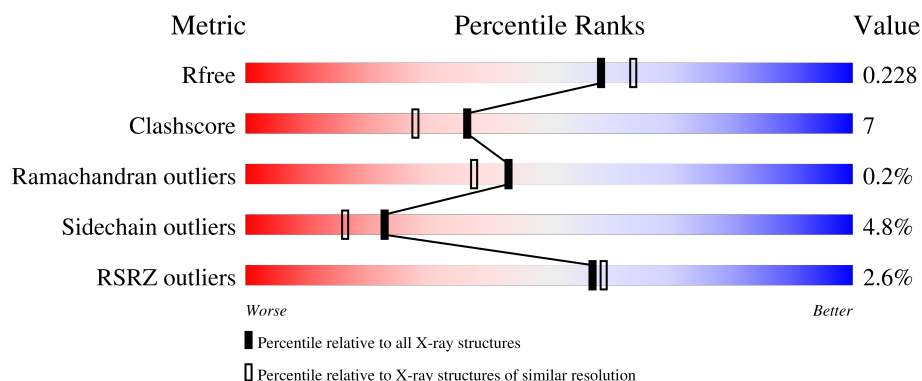
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	343	84% 10% 6%
1	B	343	85% 11% ..
1	C	343	84% 13% ..
1	D	343	75% 18% ..
1	E	343	80% 15% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	343	6% 70% 22% 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16888 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 Squalene synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2615	1663	443	491	18			
1	B	333	Total	C	N	O	S	0	0	0
			2691	1711	459	503	18			
1	C	334	Total	C	N	O	S	0	0	0
			2700	1716	459	507	18			
1	D	330	Total	C	N	O	S	0	0	0
			2673	1701	455	499	18			
1	E	329	Total	C	N	O	S	0	0	0
			2658	1692	450	498	18			
1	F	324	Total	C	N	O	S	0	0	0
			2625	1670	444	493	18			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	GLY	-	expression tag	UNP P37268
A	29	SER	-	expression tag	UNP P37268
A	30	HIS	-	expression tag	UNP P37268
B	28	GLY	-	expression tag	UNP P37268
B	29	SER	-	expression tag	UNP P37268
B	30	HIS	-	expression tag	UNP P37268
C	28	GLY	-	expression tag	UNP P37268
C	29	SER	-	expression tag	UNP P37268
C	30	HIS	-	expression tag	UNP P37268
D	28	GLY	-	expression tag	UNP P37268
D	29	SER	-	expression tag	UNP P37268
D	30	HIS	-	expression tag	UNP P37268
E	28	GLY	-	expression tag	UNP P37268
E	29	SER	-	expression tag	UNP P37268
E	30	HIS	-	expression tag	UNP P37268
F	28	GLY	-	expression tag	UNP P37268
F	29	SER	-	expression tag	UNP P37268

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	30	HIS	-	expression tag	UNP P37268

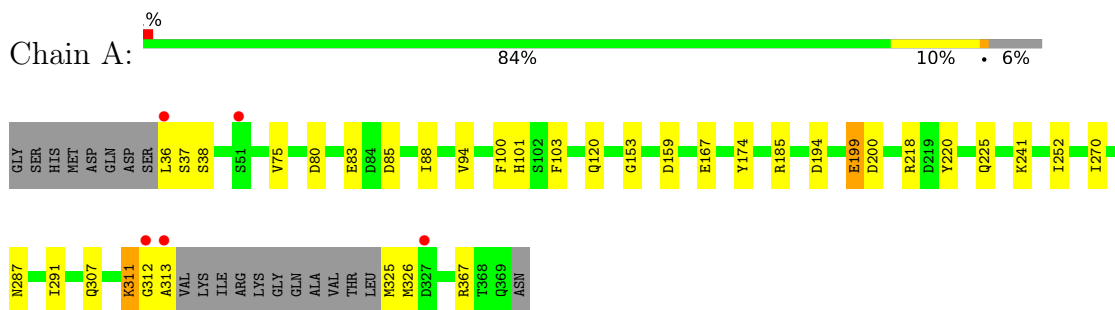
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	234	Total 234	O 234	0	0
2	B	193	Total 193	O 193	0	0
2	C	202	Total 202	O 202	0	0
2	D	82	Total 82	O 82	0	0
2	E	159	Total 159	O 159	0	0
2	F	56	Total 56	O 56	0	0

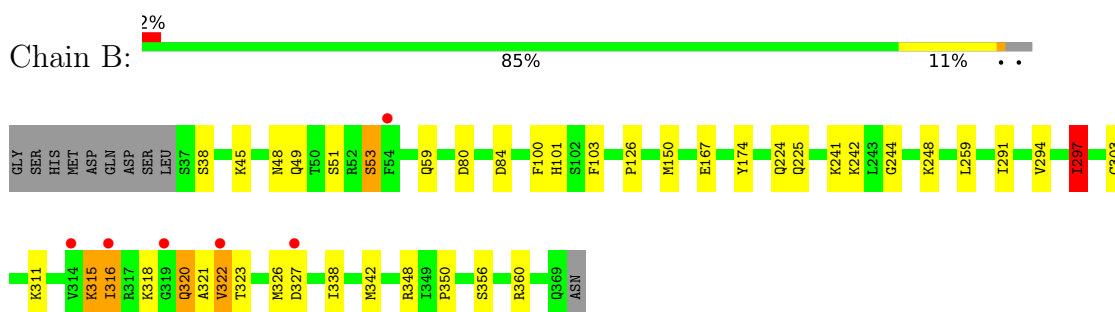
3 Residue-property plots [i](#)

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.

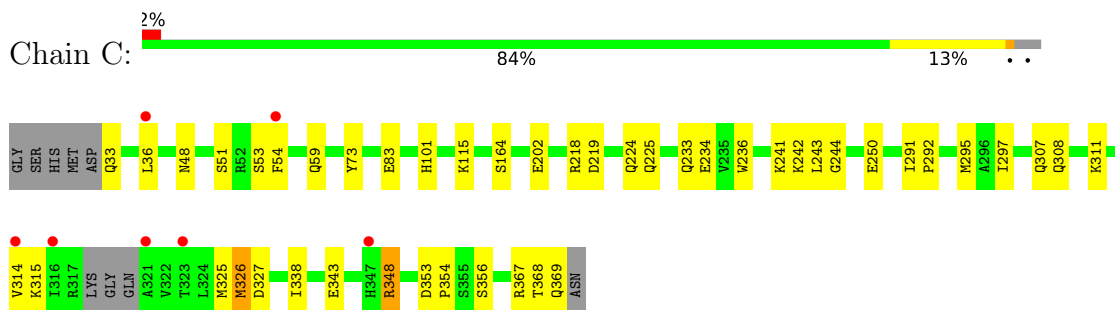
- Molecule 1: Squalene synthase



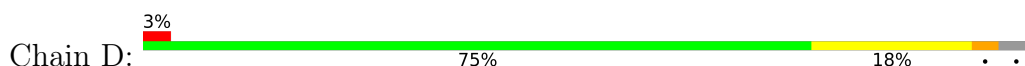
- Molecule 1: Squalene synthase

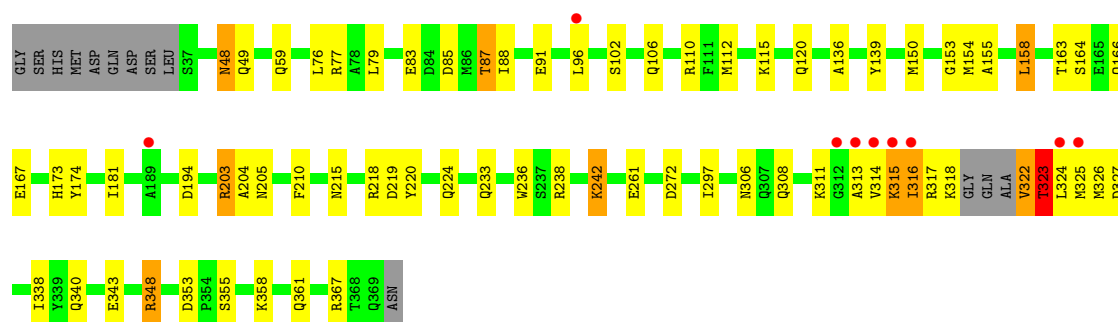


- Molecule 1: Squalene synthase

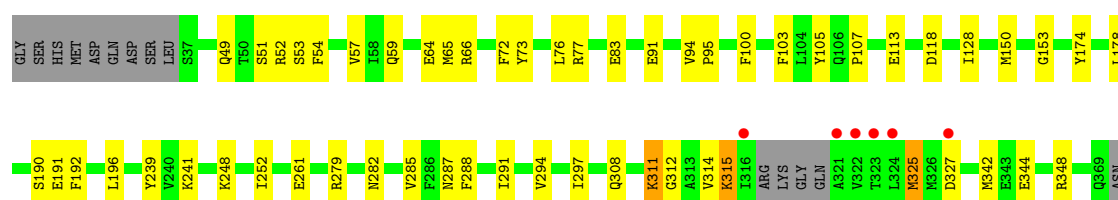
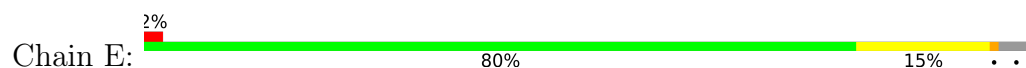


- Molecule 1: Squalene synthase

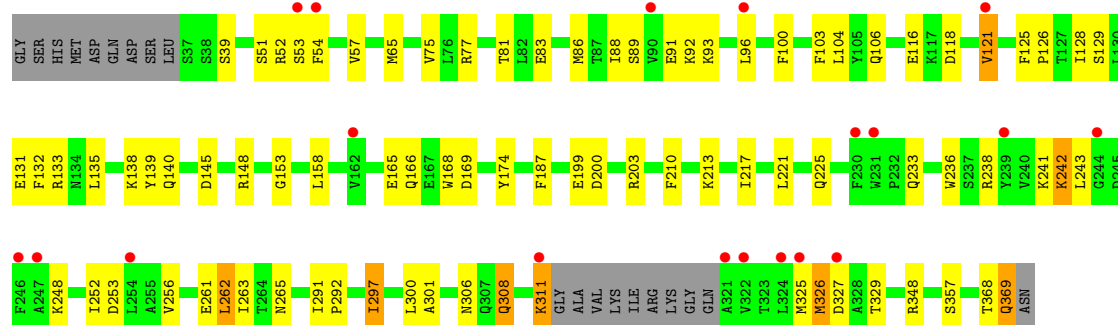




• Molecule 1: Squalene synthase



• Molecule 1: Squalene synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.61Å 153.86Å 91.52Å 90.00° 91.68° 90.00°	Depositor
Resolution (Å)	29.40 – 2.05 29.40 – 2.05	Depositor EDS
% Data completeness (in resolution range)	98.2 (29.40-2.05) 98.2 (29.40-2.05)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 2.04Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.169 , 0.227 0.170 , 0.228	Depositor DCC
R_{free} test set	7255 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	33.7	Xtriage
Anisotropy	0.734	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 61.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	16888	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 3.87% 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	0.53	0/2669	1.03	7/3609 (0.2%)
1	B	0.47	0/2746	1.00	4/3713 (0.1%)
1	C	0.49	0/2754	0.97	0/3724
1	D	0.41	0/2727	0.96	5/3686 (0.1%)
1	E	0.46	0/2712	0.98	1/3668 (0.0%)
1	F	0.38	0/2679	0.94	4/3624 (0.1%)
All	All	0.46	0/16287	0.98	21/22024 (0.1%)

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	D	0	1

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	297	ILE	CB-CA-C	-9.46	99.17	112.22
1	A	194	ASP	N-CA-CB	-6.27	100.56	110.03
1	D	323	THR	N-CA-C	-6.22	106.38	112.97
1	F	291	ILE	N-CA-CB	6.18	115.27	110.45
1	F	297	ILE	CB-CA-C	-5.94	104.37	111.97
1	A	367	ARG	CB-CG-CD	-5.86	97.82	111.30
1	A	94	VAL	N-CA-CB	5.68	114.33	110.52
1	B	248	LYS	CA-C-N	5.53	126.75	119.84
1	B	248	LYS	C-N-CA	5.53	126.75	119.84
1	A	367	ARG	CB-CA-C	-5.51	100.10	110.67
1	D	48	ASN	N-CA-C	5.39	118.07	111.82
1	D	106	GLN	CA-C-N	5.35	125.02	119.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	106	GLN	C-N-CA	5.35	125.02	119.56
1	D	314	VAL	N-CA-C	5.35	120.47	109.34
1	A	270	ILE	CA-C-N	-5.31	113.16	119.05
1	A	270	ILE	C-N-CA	-5.31	113.16	119.05
1	E	128	ILE	N-CA-C	5.28	115.49	110.42
1	A	326	MET	N-CA-C	5.24	117.98	109.24
1	F	106	GLN	CA-C-N	5.13	124.85	119.82
1	F	106	GLN	C-N-CA	5.13	124.85	119.82
1	B	297	ILE	N-CA-CB	5.07	118.19	110.58

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	313	ALA	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2615	0	2577	19	0
1	B	2691	0	2669	33	0
1	C	2700	0	2672	29	0
1	D	2673	0	2652	60	0
1	E	2658	0	2631	40	0
1	F	2625	0	2590	62	0
2	A	234	0	0	8	0
2	B	193	0	0	6	0
2	C	202	0	0	5	0
2	D	82	0	0	3	0
2	E	159	0	0	2	0
2	F	56	0	0	7	0
All	All	16888	0	15791	230	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 7.

All (230) 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:B:167:GLU:HG2	2:B:1056:HOH:O	1.43	1.13
1:E:297:ILE:HD11	1:E:342:MET:CE	1.84	1.06
1:A:325:MET:O	1:C:327:ASP:HB2	1.56	1.02
1:D:83:GLU:HB2	1:D:154:MET:HE3	1.46	0.98
1:F:132:PHE:O	2:F:954:HOH:O	1.81	0.98
1:C:54:PHE:HA	2:C:1175:HOH:O	1.64	0.97
1:F:213:LYS:O	1:F:217:ILE:HG12	1.66	0.95
1:E:297:ILE:HD11	1:E:342:MET:HE3	1.48	0.93
1:B:315:LYS:H	1:B:315:LYS:HD3	1.35	0.90
1:C:48:ASN:HD21	1:C:59:GLN:HE22	1.18	0.88
1:D:48:ASN:HD21	1:D:59:GLN:HE22	1.22	0.85
1:F:65:MET:CE	1:F:187:PHE:HD1	1.91	0.83
1:E:64:GLU:HG2	2:E:1302:HOH:O	1.79	0.83
1:D:315:LYS:HD2	1:D:315:LYS:O	1.79	0.81
1:F:65:MET:HE1	1:F:187:PHE:CD1	2.15	0.81
1:D:348:ARG:HH11	1:D:348:ARG:HG2	1.48	0.78
1:E:297:ILE:CD1	1:E:342:MET:HE3	2.13	0.78
1:B:291:ILE:HD11	1:C:326:MET:HE3	1.66	0.77
1:D:163:THR:HG22	1:D:164:SER:N	1.99	0.77
1:F:65:MET:CE	1:F:187:PHE:CD1	2.70	0.75
1:D:322:VAL:HG12	1:D:324:LEU:HB2	1.69	0.74
1:F:327:ASP:OD2	2:F:905:HOH:O	2.06	0.74
1:F:88:ILE:HG22	1:F:93:LYS:HG3	1.70	0.74
1:D:325:MET:O	1:F:327:ASP:HB2	1.87	0.73
1:E:297:ILE:CD1	1:E:342:MET:CE	2.64	0.73
1:B:297:ILE:CG2	1:B:342:MET:HE1	2.19	0.72
1:A:80:ASP:OD1	2:A:1166:HOH:O	2.07	0.72
1:B:297:ILE:CG2	1:B:342:MET:CE	2.67	0.72
1:B:297:ILE:HG21	1:B:342:MET:CE	2.19	0.72
1:F:135:LEU:HB2	2:F:954:HOH:O	1.90	0.72
1:B:84:ASP:OD1	2:B:884:HOH:O	2.08	0.71
1:F:88:ILE:CG2	1:F:93:LYS:HG3	2.19	0.71
1:D:85:ASP:HB3	1:D:88:ILE:HD12	1.71	0.71
1:D:322:VAL:HG12	1:D:324:LEU:CB	2.21	0.71
1:F:54:PHE:CE1	1:F:57:VAL:HG21	2.24	0.71
1:B:323:THR:HA	1:B:326:MET:HE3	1.73	0.70
1:D:343:GLU:OE2	1:D:367:ARG:HD3	1.91	0.70
1:D:167:GLU:HG2	2:D:1205:HOH:O	1.91	0.69
1:D:297:ILE:HD13	1:D:338:ILE:HG12	1.73	0.69
1:F:210:PHE:HZ	1:F:297:ILE:HD13	1.59	0.68
1:D:323:THR:HG23	1:D:323:THR:O	1.91	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:291:ILE:HD11	1:F:326:MET:HE3	1.76	0.67
1:C:48:ASN:HD21	1:C:59:GLN:NE2	1.91	0.66
1:E:282:ASN:HD22	1:E:285:VAL:H	1.42	0.66
1:A:83:GLU:OE1	2:A:1166:HOH:O	2.14	0.66
1:A:200:ASP:HB3	2:A:1310:HOH:O	1.96	0.65
1:B:51:SER:HB2	2:B:1280:HOH:O	1.97	0.65
1:F:129:SER:HB3	1:F:133:ARG:HH12	1.61	0.65
1:A:101:HIS:HE1	2:A:794:HOH:O	1.78	0.65
1:E:77:ARG:HD2	1:E:118:ASP:OD2	1.98	0.64
1:B:291:ILE:CD1	1:C:326:MET:HE3	2.28	0.63
1:F:140:GLN:CG	2:F:954:HOH:O	2.46	0.63
1:D:83:GLU:HB2	1:D:154:MET:CE	2.24	0.63
1:F:369:GLN:O	1:F:369:GLN:NE2	2.30	0.62
1:C:348:ARG:HG3	1:C:348:ARG:HH11	1.65	0.62
1:D:203:ARG:NH2	1:D:272:ASP:OD1	2.32	0.62
1:B:48:ASN:HD21	1:B:59:GLN:HE22	1.48	0.62
1:C:202:GLU:HB3	2:C:1247:HOH:O	2.00	0.61
1:D:49:GLN:HE21	1:D:120:GLN:HE21	1.48	0.61
1:D:323:THR:H	1:D:340:GLN:NE2	1.97	0.60
1:E:57:VAL:HG11	1:E:288:PHE:HA	1.83	0.60
1:D:48:ASN:HD21	1:D:59:GLN:NE2	1.97	0.60
1:E:327:ASP:OD2	1:F:326:MET:HA	2.01	0.60
1:D:324:LEU:HD12	1:D:326:MET:H	1.66	0.59
1:F:129:SER:HB3	1:F:133:ARG:NH1	2.17	0.59
1:D:83:GLU:CB	1:D:154:MET:HE3	2.25	0.59
1:D:323:THR:H	1:D:340:GLN:HE22	1.49	0.59
1:A:311:LYS:HB2	1:A:311:LYS:NZ	2.18	0.59
1:D:306:ASN:HD21	1:D:315:LYS:HZ1	1.51	0.58
1:B:297:ILE:HG21	1:B:342:MET:HE3	1.85	0.57
1:F:145:ASP:OD1	1:F:148:ARG:NH2	2.37	0.57
1:E:51:SER:C	1:E:53:SER:H	2.11	0.57
1:A:307:GLN:HG2	2:A:697:HOH:O	2.03	0.57
1:E:59:GLN:O	1:E:66:ARG:HD2	2.05	0.57
1:D:348:ARG:HH11	1:D:348:ARG:CG	2.17	0.57
1:C:308:GLN:HA	1:C:311:LYS:HG2	1.87	0.56
1:F:118:ASP:O	1:F:121:VAL:HG12	2.05	0.56
1:C:218:ARG:NH1	1:C:219:ASP:OD1	2.39	0.56
1:F:39:SER:OG	1:F:131:GLU:OE2	2.21	0.56
1:C:101:HIS:HE1	2:C:968:HOH:O	1.88	0.55
1:E:344:GLU:O	1:E:348:ARG:HG3	2.06	0.55
1:D:181:ILE:HD13	1:D:204:ALA:HB3	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:306:ASN:HD21	1:D:315:LYS:NZ	2.05	0.55
1:A:185:ARG:NH2	2:A:1117:HOH:O	2.29	0.55
1:D:308:GLN:NE2	1:D:315:LYS:NZ	2.55	0.55
1:F:241:LYS:C	1:F:242:LYS:HD2	2.32	0.55
1:D:324:LEU:HD11	1:D:326:MET:O	2.07	0.54
1:E:51:SER:O	1:E:53:SER:N	2.41	0.54
1:A:312:GLY:O	1:A:313:ALA:HB2	2.08	0.54
1:E:315:LYS:HE3	1:E:315:LYS:H	1.73	0.54
1:D:163:THR:CG2	1:D:164:SER:N	2.69	0.54
1:B:320:GLN:H	1:B:320:GLN:CD	2.15	0.54
1:F:210:PHE:CZ	1:F:297:ILE:HD13	2.42	0.53
1:E:327:ASP:HB2	1:F:325:MET:O	2.08	0.53
1:F:263:ILE:HG23	1:F:300:LEU:HG	1.91	0.53
1:C:54:PHE:CA	2:C:1175:HOH:O	2.39	0.53
1:F:65:MET:HE3	1:F:187:PHE:HA	1.90	0.53
1:D:150:MET:HB2	1:D:174:TYR:O	2.08	0.53
1:A:287:ASN:O	1:A:291:ILE:HG12	2.09	0.53
1:E:311:LYS:HB2	1:E:311:LYS:NZ	2.23	0.52
1:F:238:ARG:NH2	1:F:261:GLU:OE2	2.40	0.52
1:C:51:SER:HB2	1:C:73:TYR:CZ	2.44	0.52
1:F:121:VAL:HG23	1:F:128:ILE:HD13	1.92	0.52
1:B:327:ASP:OD2	1:C:327:ASP:OD1	2.28	0.52
1:C:233:GLN:HA	1:C:236:TRP:NE1	2.25	0.52
1:D:155:ALA:HA	1:D:158:LEU:HD22	1.92	0.52
1:C:33:GLN:HB3	1:C:36:LEU:HG	1.92	0.51
1:C:343:GLU:OE1	1:C:367:ARG:NH2	2.41	0.51
1:C:348:ARG:NH1	2:C:699:HOH:O	2.43	0.51
1:A:218:ARG:NH1	2:A:772:HOH:O	2.36	0.51
1:B:101:HIS:HD2	2:B:855:HOH:O	1.92	0.51
1:E:65:MET:HE2	1:E:192:PHE:CD2	2.45	0.51
1:F:83:GLU:HG2	2:F:1126:HOH:O	2.09	0.51
1:E:239:TYR:OH	1:E:261:GLU:OE1	2.21	0.51
1:F:51:SER:O	1:F:52:ARG:C	2.53	0.51
1:D:163:THR:HG22	1:D:164:SER:H	1.71	0.51
1:B:150:MET:HG3	1:B:174:TYR:O	2.09	0.51
1:F:233:GLN:HA	1:F:236:TRP:CD1	2.46	0.51
1:F:233:GLN:HA	1:F:236:TRP:NE1	2.26	0.51
1:B:48:ASN:HD21	1:B:59:GLN:NE2	2.09	0.50
1:D:353:ASP:OD1	2:D:757:HOH:O	2.20	0.50
1:F:253:ASP:O	1:F:256:VAL:HG12	2.10	0.50
1:B:100:PHE:HA	1:B:103:PHE:CD2	2.47	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:210:PHE:CE2	1:D:297:ILE:HG13	2.46	0.50
1:F:327:ASP:OD1	1:F:327:ASP:C	2.55	0.50
1:D:327:ASP:HB2	1:E:325:MET:O	2.12	0.49
1:E:53:SER:OG	1:E:54:PHE:N	2.45	0.49
1:A:120:GLN:HB2	2:A:1014:HOH:O	2.12	0.49
1:A:311:LYS:HB2	1:A:311:LYS:HZ2	1.77	0.49
1:E:100:PHE:HA	1:E:103:PHE:CD2	2.47	0.49
1:B:356:SER:O	1:B:360:ARG:HG3	2.11	0.49
1:C:292:PRO:HA	1:C:295:MET:HE2	1.94	0.49
1:D:308:GLN:HE22	1:D:315:LYS:NZ	2.11	0.49
1:D:166:GLN:H	1:D:166:GLN:CD	2.19	0.49
1:A:100:PHE:HA	1:A:103:PHE:CD2	2.48	0.49
1:F:368:THR:O	1:F:369:GLN:C	2.56	0.49
1:B:322:VAL:O	1:B:326:MET:HE2	2.12	0.49
1:A:85:ASP:HB3	1:A:88:ILE:HD12	1.94	0.49
1:D:324:LEU:CD1	1:D:326:MET:HB2	2.43	0.49
1:E:196:LEU:HD21	1:E:279:ARG:CZ	2.43	0.48
1:E:294:VAL:O	1:E:297:ILE:HG22	2.13	0.48
1:C:291:ILE:HB	1:C:292:PRO:HD3	1.96	0.48
1:D:315:LYS:HD3	1:D:317:ARG:HH21	1.78	0.48
1:E:190:SER:O	1:E:191:GLU:HB2	2.12	0.48
1:F:168:TRP:CZ3	1:F:213:LYS:HE3	2.49	0.48
1:D:322:VAL:CG1	1:D:324:LEU:HB2	2.42	0.48
1:D:236:TRP:CZ3	1:D:242:LYS:HA	2.49	0.47
1:D:79:LEU:HG	1:D:154:MET:HE1	1.96	0.47
1:B:80:ASP:OD1	2:B:884:HOH:O	2.20	0.47
1:B:323:THR:HA	1:B:326:MET:CE	2.40	0.47
1:A:153:GLY:HA3	1:A:174:TYR:CG	2.49	0.47
1:D:324:LEU:CD1	1:D:326:MET:O	2.62	0.47
1:C:348:ARG:HG3	1:C:348:ARG:NH1	2.28	0.46
1:F:221:LEU:O	1:F:225:GLN:HG2	2.16	0.46
1:F:301:ALA:O	1:F:348:ARG:NH2	2.48	0.46
1:B:315:LYS:HD3	1:B:315:LYS:N	2.15	0.46
1:F:77:ARG:HA	1:F:77:ARG:HD2	1.76	0.46
1:E:72:PHE:CZ	1:E:76:LEU:HD11	2.52	0.45
1:F:75:VAL:HG11	1:F:104:LEU:HD21	1.97	0.45
1:F:88:ILE:HG21	1:F:93:LYS:HG3	1.96	0.45
1:D:316:ILE:H	1:D:316:ILE:HG13	1.57	0.45
1:F:308:GLN:HA	1:F:311:LYS:HD3	1.99	0.45
1:B:53:SER:HB2	2:B:1249:HOH:O	2.16	0.45
1:F:54:PHE:CE1	1:F:57:VAL:CG2	2.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:ILE:HG22	1:B:342:MET:HE1	1.94	0.44
1:D:233:GLN:HA	1:D:236:TRP:NE1	2.32	0.44
1:E:311:LYS:HZ2	1:E:312:GLY:H	1.65	0.44
1:D:323:THR:HG22	1:D:340:GLN:HE22	1.82	0.44
1:E:105:TYR:O	1:E:107:PRO:HD3	2.17	0.44
1:D:136:ALA:HB3	1:D:139:TYR:CD2	2.52	0.44
1:E:287:ASN:ND2	1:F:326:MET:HE1	2.33	0.44
1:F:327:ASP:OD1	1:F:329:THR:OG1	2.27	0.44
1:D:210:PHE:HE2	1:D:297:ILE:HG13	1.83	0.43
1:C:224:GLN:NE2	1:C:244:GLY:HA2	2.33	0.43
1:F:140:GLN:HG2	2:F:954:HOH:O	2.16	0.43
1:D:308:GLN:NE2	1:D:315:LYS:HZ1	2.16	0.43
1:E:57:VAL:CG1	1:E:288:PHE:HA	2.47	0.43
1:B:51:SER:O	1:B:51:SER:OG	2.36	0.43
1:E:51:SER:C	1:E:53:SER:N	2.76	0.43
1:E:94:VAL:HB	1:E:95:PRO:HD3	2.00	0.43
1:C:233:GLN:HA	1:C:236:TRP:CD1	2.54	0.43
1:D:238:ARG:NH2	1:D:261:GLU:OE2	2.52	0.43
1:B:294:VAL:HG11	1:C:325:MET:HE2	2.00	0.43
1:D:224:GLN:HG2	2:D:879:HOH:O	2.19	0.43
1:B:259:LEU:HD21	1:B:303:CYS:O	2.19	0.42
1:F:121:VAL:HG23	1:F:128:ILE:CD1	2.47	0.42
1:F:140:GLN:HG3	2:F:954:HOH:O	2.14	0.42
1:B:45:LYS:O	1:B:49:GLN:HG3	2.18	0.42
1:E:49:GLN:NE2	2:E:1211:HOH:O	2.53	0.42
1:D:153:GLY:HA3	1:D:174:TYR:CG	2.54	0.42
1:E:153:GLY:HA3	1:E:174:TYR:CG	2.54	0.42
1:D:85:ASP:OD1	1:D:87:THR:HB	2.19	0.42
1:B:297:ILE:HD13	1:B:338:ILE:HA	2.02	0.42
1:F:65:MET:HE3	1:F:187:PHE:HD1	1.78	0.42
1:D:326:MET:HA	1:F:327:ASP:HB2	2.01	0.42
1:B:348:ARG:O	1:B:350:PRO:HD3	2.19	0.42
1:C:164:SER:HA	1:C:234:GLU:HB2	2.02	0.42
1:E:314:VAL:HA	1:E:315:LYS:HE3	2.02	0.42
1:A:252:ILE:HD11	1:A:307:GLN:HB2	2.02	0.41
1:D:219:ASP:O	1:D:220:TYR:C	2.63	0.41
1:F:138:LYS:HE3	1:F:139:TYR:CZ	2.54	0.41
1:D:173:HIS:HD2	1:D:205:ASN:OD1	2.03	0.41
1:A:199:GLU:HG2	1:E:196:LEU:HD22	2.02	0.41
1:B:224:GLN:NE2	1:B:244:GLY:HA2	2.35	0.41
1:B:297:ILE:H	1:B:297:ILE:HG13	1.67	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:262:LEU:O	1:F:265:ASN:HB3	2.21	0.41
1:D:110:ARG:HD3	1:D:112:MET:SD	2.61	0.41
1:E:73:TYR:CD2	1:E:73:TYR:C	2.98	0.41
1:E:308:GLN:HB3	1:E:314:VAL:HG22	2.02	0.41
1:F:86:MET:HA	1:F:86:MET:HE2	2.03	0.41
1:A:220:TYR:CD2	1:A:220:TYR:C	2.99	0.41
1:C:297:ILE:HD13	1:C:338:ILE:HG12	2.02	0.41
1:C:353:ASP:HA	1:C:354:PRO:HD3	1.85	0.41
1:F:89:SER:HB3	1:F:92:LYS:HE3	2.03	0.41
1:F:153:GLY:HA3	1:F:174:TYR:CG	2.55	0.41
1:F:200:ASP:OD2	1:F:203:ARG:HB2	2.21	0.41
1:D:215:ASN:OD1	1:D:218:ARG:NH2	2.54	0.41
1:D:322:VAL:HG12	1:D:324:LEU:HB3	2.00	0.41
1:D:324:LEU:HD12	1:D:326:MET:N	2.33	0.41
1:E:174:TYR:HA	1:E:178:LEU:HD12	2.04	0.41
1:F:100:PHE:HA	1:F:103:PHE:CD2	2.55	0.41
1:F:306:ASN:OD1	1:F:308:GLN:N	2.52	0.41
1:C:236:TRP:CE2	1:C:243:LEU:HB2	2.56	0.40
1:F:125:PHE:N	1:F:126:PRO:CD	2.84	0.40
1:F:213:LYS:HE2	1:F:265:ASN:OD1	2.22	0.40
1:E:150:MET:HE3	1:E:150:MET:HB2	1.90	0.40
1:F:54:PHE:CE1	1:F:292:PRO:HG3	2.56	0.40
1:C:353:ASP:HB3	1:C:356:SER:HB3	2.03	0.40
1:D:348:ARG:CG	1:D:348:ARG:NH1	2.82	0.40
1:F:81:THR:HG23	1:F:116:GLU:HG2	2.02	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	319/343 (93%)	313 (98%)	6 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	331/343 (96%)	321 (97%)	8 (2%)	2 (1%)	21	13
1	C	330/343 (96%)	321 (97%)	8 (2%)	1 (0%)	36	30
1	D	326/343 (95%)	314 (96%)	12 (4%)	0	100	100
1	E	325/343 (95%)	314 (97%)	10 (3%)	1 (0%)	36	30
1	F	320/343 (93%)	304 (95%)	16 (5%)	0	100	100
All	All	1951/2058 (95%)	1887 (97%)	60 (3%)	4 (0%)	43	37

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	316	ILE
1	E	52	ARG
1	B	321	ALA
1	C	314	VAL

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	288/305 (94%)	278 (96%)	10 (4%)	32	27
1	B	296/305 (97%)	283 (96%)	13 (4%)	25	19
1	C	298/305 (98%)	285 (96%)	13 (4%)	25	19
1	D	295/305 (97%)	274 (93%)	21 (7%)	13	7
1	E	293/305 (96%)	284 (97%)	9 (3%)	35	30
1	F	290/305 (95%)	271 (93%)	19 (7%)	15	9
All	All	1760/1830 (96%)	1675 (95%)	85 (5%)	23	16

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LEU
1	A	37	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	38	SER
1	A	75	VAL
1	A	159	ASP
1	A	167	GLU
1	A	199	GLU
1	A	225	GLN
1	A	241	LYS
1	A	311	LYS
1	B	38	SER
1	B	53	SER
1	B	126	PRO
1	B	225	GLN
1	B	241	LYS
1	B	242	LYS
1	B	297	ILE
1	B	311	LYS
1	B	315	LYS
1	B	316	ILE
1	B	318	LYS
1	B	320	GLN
1	B	322	VAL
1	C	53	SER
1	C	83	GLU
1	C	115	LYS
1	C	225	GLN
1	C	241	LYS
1	C	242	LYS
1	C	250	GLU
1	C	307	GLN
1	C	315	LYS
1	C	326	MET
1	C	348	ARG
1	C	368	THR
1	C	369	GLN
1	D	76	LEU
1	D	77	ARG
1	D	87	THR
1	D	91	GLU
1	D	96	LEU
1	D	102	SER
1	D	115	LYS
1	D	158	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	194	ASP
1	D	203	ARG
1	D	242	LYS
1	D	311	LYS
1	D	315	LYS
1	D	316	ILE
1	D	318	LYS
1	D	322	VAL
1	D	323	THR
1	D	348	ARG
1	D	355	SER
1	D	358	LYS
1	D	361	GLN
1	E	83	GLU
1	E	91	GLU
1	E	113	GLU
1	E	241	LYS
1	E	248	LYS
1	E	252	ILE
1	E	311	LYS
1	E	315	LYS
1	E	325	MET
1	F	53	SER
1	F	91	GLU
1	F	96	LEU
1	F	121	VAL
1	F	158	LEU
1	F	165	GLU
1	F	166	GLN
1	F	169	ASP
1	F	199	GLU
1	F	242	LYS
1	F	243	LEU
1	F	248	LYS
1	F	252	ILE
1	F	262	LEU
1	F	308	GLN
1	F	311	LYS
1	F	326	MET
1	F	357	SER
1	F	369	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	A	225	GLN
1	A	251	ASN
1	A	287	ASN
1	A	307	GLN
1	B	48	ASN
1	B	59	GLN
1	B	99	ASN
1	B	101	HIS
1	B	224	GLN
1	B	308	GLN
1	B	347	HIS
1	C	48	ASN
1	C	59	GLN
1	C	101	HIS
1	C	224	GLN
1	C	251	ASN
1	C	283	GLN
1	C	293	GLN
1	C	307	GLN
1	D	48	ASN
1	D	49	GLN
1	D	98	HIS
1	D	101	HIS
1	D	161	HIS
1	D	173	HIS
1	D	224	GLN
1	D	251	ASN
1	D	257	GLN
1	D	306	ASN
1	D	308	GLN
1	D	340	GLN
1	E	49	GLN
1	E	67	ASN
1	E	98	HIS
1	E	140	GLN
1	E	251	ASN
1	E	282	ASN
1	E	308	GLN
1	E	340	GLN
1	E	361	GLN
1	F	48	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	49	GLN
1	F	59	GLN
1	F	98	HIS
1	F	101	HIS
1	F	106	GLN
1	F	120	GLN
1	F	140	GLN
1	F	305	ASN
1	F	308	GLN
1	F	340	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	323/343 (94%)	-0.40	5 (1%) 72 73	24, 35, 60, 75	0
1	B	333/343 (97%)	-0.18	6 (1%) 67 69	29, 41, 78, 98	0
1	C	334/343 (97%)	-0.20	7 (2%) 63 65	25, 39, 85, 108	0
1	D	330/343 (96%)	0.17	9 (2%) 56 58	38, 59, 98, 116	0
1	E	329/343 (95%)	-0.10	6 (1%) 67 69	28, 47, 89, 104	0
1	F	324/343 (94%)	0.42	19 (5%) 28 28	34, 72, 117, 136	0
All	All	1973/2058 (95%)	-0.05	52 (2%) 57 59	24, 48, 97, 136	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	322	VAL	3.8
1	C	314	VAL	3.8
1	E	321	ALA	3.7
1	F	54	PHE	3.7
1	D	316	ILE	3.5
1	F	230	PHE	3.5
1	E	323	THR	3.4
1	B	319	GLY	3.4
1	D	314	VAL	3.2
1	D	312	GLY	3.2
1	C	323	THR	3.1
1	A	313	ALA	3.1
1	C	316	ILE	3.1
1	D	325	MET	3.0
1	F	247	ALA	3.0
1	F	90	VAL	3.0
1	F	322	VAL	3.0
1	F	321	ALA	2.9
1	C	321	ALA	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	324	LEU	2.7
1	F	53	SER	2.7
1	A	327	ASP	2.7
1	A	36	LEU	2.7
1	D	313	ALA	2.6
1	F	244	GLY	2.6
1	F	231	TRP	2.6
1	D	324	LEU	2.6
1	B	314	VAL	2.6
1	F	162	VAL	2.6
1	F	239	TYR	2.5
1	F	254	LEU	2.5
1	F	324	LEU	2.5
1	A	312	GLY	2.5
1	B	316	ILE	2.5
1	E	316	ILE	2.5
1	D	189	ALA	2.4
1	C	36	LEU	2.4
1	A	51	SER	2.4
1	F	327	ASP	2.4
1	F	325	MET	2.3
1	D	96	LEU	2.3
1	F	96	LEU	2.3
1	B	322	VAL	2.2
1	F	121	VAL	2.2
1	C	347	HIS	2.2
1	F	311	LYS	2.2
1	C	54	PHE	2.1
1	F	246	PHE	2.1
1	E	327	ASP	2.1
1	B	54	PHE	2.1
1	B	327	ASP	2.0
1	D	315	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

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.