Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:56 PM GMT

PDB ID	:	3VJB
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

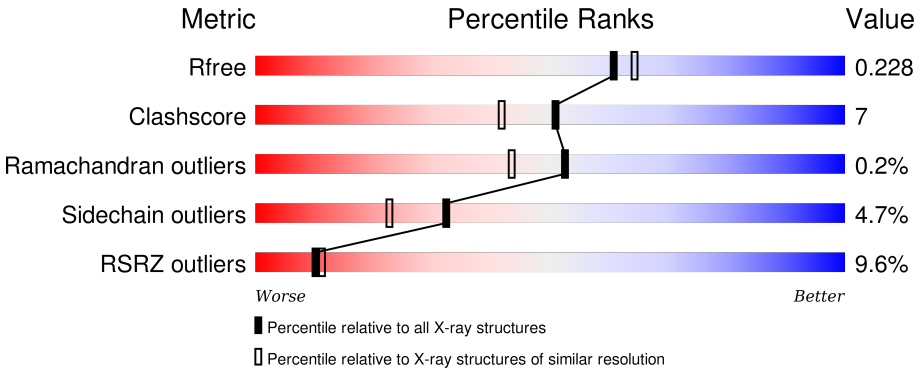
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 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}	91344	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	85% 8% • 6%
1	B	343	7% 85% 10% • •
1	C	343	7% 84% 13% • •
1	D	343	9% 76% 18% • •
1	E	343	11% 82% 12% • •

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Mol	Chain	Length	Quality of chain
1	F	343	

2 Entry composition (i)

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

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Chain	Residue	Modelled	Actual	Comment	Reference
F	30	HIS	-	EXPRESSION TAG	UNP P37268

- Molecule 2 is water.

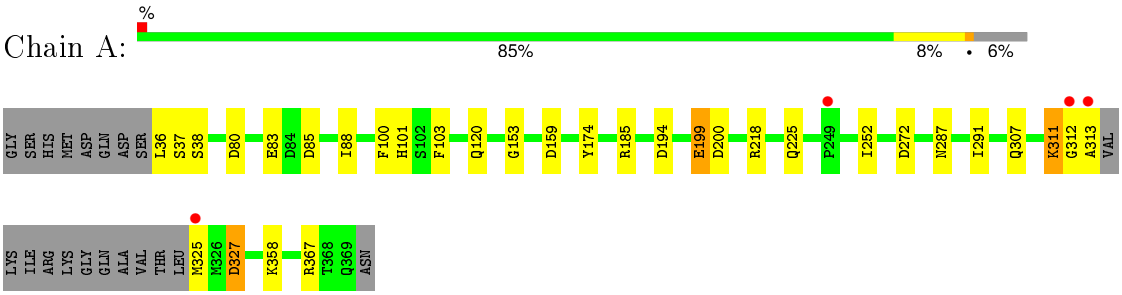
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	234	Total O 234 234	0	0
2	B	193	Total O 193 193	0	0
2	C	202	Total O 202 202	0	0
2	D	82	Total O 82 82	0	0
2	E	159	Total O 159 159	0	0
2	F	56	Total O 56 56	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

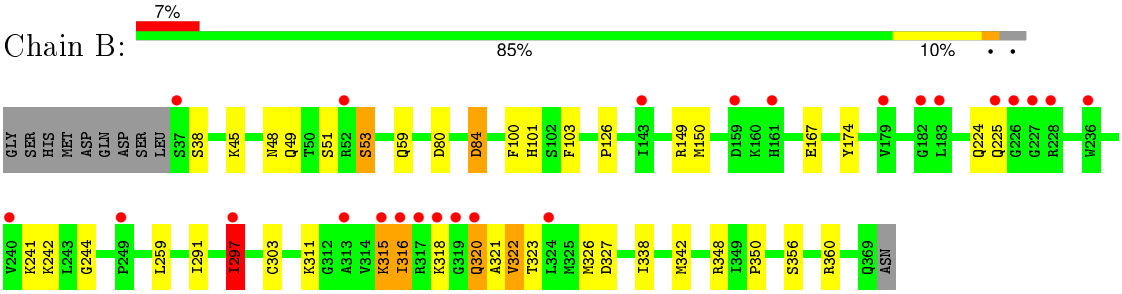
- Molecule 1: Squalene synthase

Chain A:



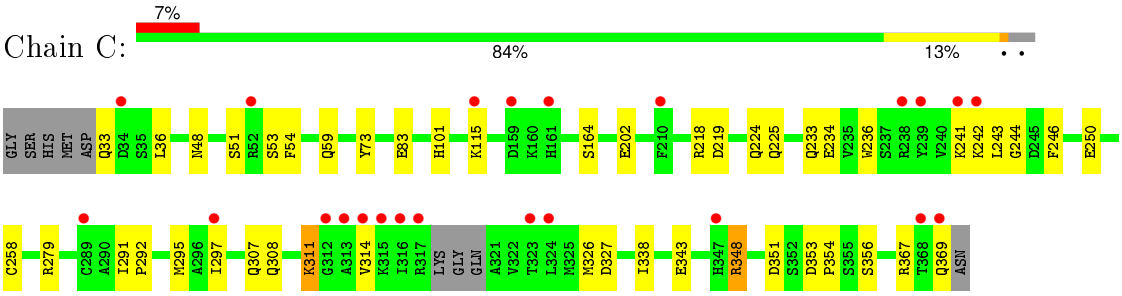
- Molecule 1: Squalene synthase

Chain B:



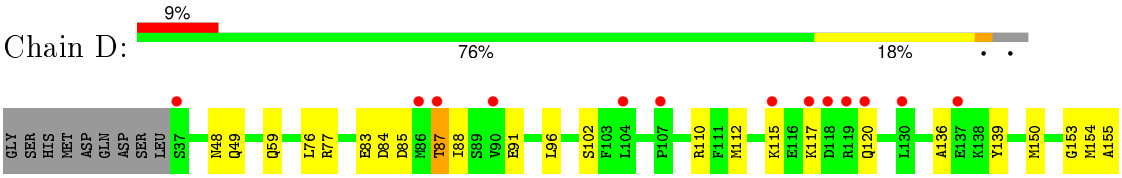
- Molecule 1: Squalene synthase

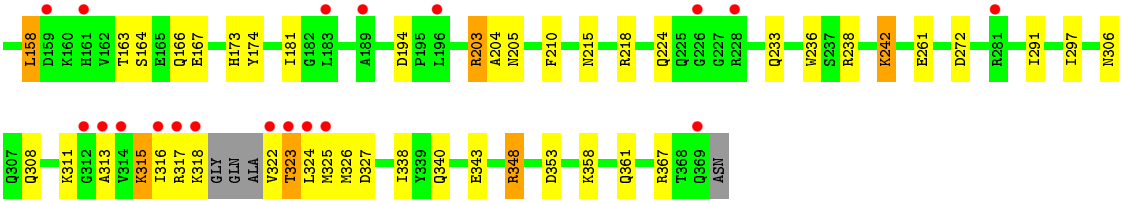
Chain C:



- Molecule 1: Squalene synthase

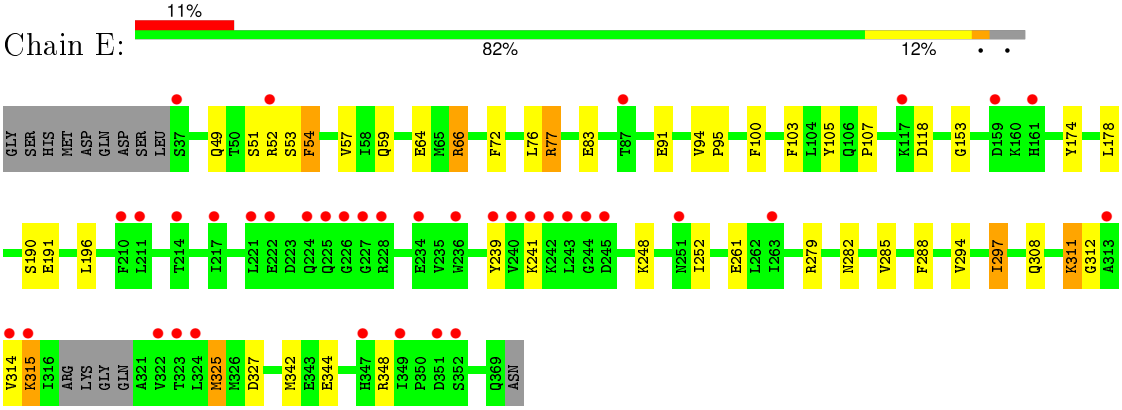
Chain D:





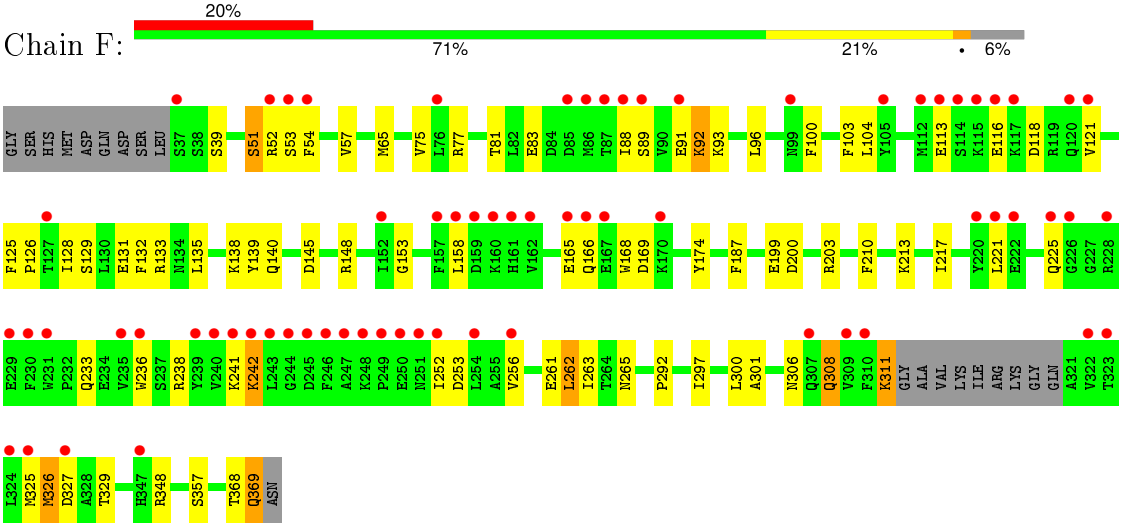
- Molecule 1: Squalene synthase

Chain E:



- Molecule 1: Squalene synthase

Chain F:



4 Data and refinement statistics (i)

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 29.44 – 2.05	Depositor EDS
% Data completeness (in resolution range)	98.2 (29.40-2.05) 98.2 (29.44-2.05)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.65 (at 2.04Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.169 , 0.227 0.169 , 0.228	Depositor DCC
R_{free} test set	7255 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	33.7	Xtriage
Anisotropy	0.734	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 54.3	EDS
Estimated twinning fraction	0.024 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 144833 reflections	Xtriage
F_o,F_c correlation	0.96	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.45	0/2669	0.78	5/3609 (0.1%)
1	B	0.38	0/2746	0.71	3/3713 (0.1%)
1	C	0.41	0/2754	0.72	1/3724 (0.0%)
1	D	0.33	0/2727	0.64	1/3686 (0.0%)
1	E	0.38	0/2712	0.69	2/3668 (0.1%)
1	F	0.30	0/2679	0.61	0/3624
All	All	0.38	0/16287	0.69	12/22024 (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 (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	297	ILE	CB-CA-C	-6.22	99.17	111.60
1	E	66	ARG	NE-CZ-NH1	-6.11	117.25	120.30
1	A	194	ASP	N-CA-CB	-5.58	100.56	110.60
1	C	279	ARG	NE-CZ-NH1	-5.46	117.57	120.30
1	A	272	ASP	CB-CG-OD1	5.41	123.17	118.30
1	A	327	ASP	CB-CG-OD1	5.34	123.11	118.30
1	E	297	ILE	CG1-CB-CG2	-5.31	99.72	111.40
1	A	367	ARG	CB-CG-CD	-5.30	97.82	111.60
1	D	291	ILE	CG1-CB-CG2	-5.30	99.75	111.40
1	B	149	ARG	NE-CZ-NH1	-5.17	117.72	120.30
1	A	367	ARG	CB-CA-C	-5.15	100.10	110.40
1	B	84	ASP	CB-CA-C	-5.01	100.38	110.40

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 (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	2615	0	2577	18	0
1	B	2691	0	2669	29	0
1	C	2700	0	2672	29	0
1	D	2673	0	2652	57	0
1	E	2658	0	2631	36	0
1	F	2625	0	2590	59	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	219	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 (219) 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: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:B:315:LYS:H	1:B:315:LYS:HD3	1.35	0.90
1:E:297:ILE:HD11	1:E:342:MET:HE3	1.52	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:348:ARG:HH11	1:D:348:ARG:HG2	1.48	0.78
1:F:65:MET:HE1	1:F:187:PHE:CD1	2.18	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:B:297:ILE:CG2	1:B:342:MET:HE1	2.15	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:CE	2.67	0.72
1:A:80:ASP:OD1	2:A:1166:HOH:O	2.07	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:322:VAL:HG12	1:D:324:LEU:CB	2.21	0.71
1:D:85:ASP:HB3	1:D:88:ILE:HD12	1.71	0.71
1:F:54:PHE:CE1	1:F:57:VAL:HG21	2.24	0.71
1:F:65:MET:HE1	1:F:187:PHE:HD1	1.53	0.71
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:D:83:GLU:HB2	1:D:154:MET:HE2	1.75	0.68
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
1:D:83:GLU:HB2	1:D:154:MET:CE	2.24	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:F:129:SER:HB3	1:F:133:ARG:HH12	1.61	0.65
1:B:51:SER:HB2	2:B:1280:HOH:O	1.97	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:F:140:GLN:CG	2:F:954:HOH:O	2.46	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:369:GLN:NE2	1:F:369:GLN:O	2.30	0.62
1:D:203:ARG:NH2	1:D:272:ASP:OD1	2.32	0.62
1:C:348:ARG:HH11	1:C:348:ARG:HG3	1.65	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:323:THR:H	1:D:340:GLN:HE22	1.49	0.59
1:D:306:ASN:HD21	1:D:315:LYS:HZ1	1.49	0.59
1:A:311:LYS:NZ	1:A:311:LYS:HB2	2.18	0.59
1:E:297:ILE:CD1	1:E:342:MET:HE1	2.33	0.58
1:F:145:ASP:OD1	1:F:148:ARG:NH2	2.37	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:297:ILE:CD1	1:E:342:MET:HE3	2.28	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
1:D:306:ASN:HD21	1:D:315:LYS:NZ	2.05	0.55
1:D:308:GLN:NE2	1:D:315:LYS:NZ	2.55	0.55
1:A:185:ARG:NH2	2:A:1117:HOH:O	2.29	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:E:297:ILE:HD11	1:E:342:MET:HE1	1.81	0.54
1:D:163:THR:CG2	1:D:164:SER:N	2.69	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:51:SER:C	1:E:53:SER:H	2.11	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:NZ	1:E:311:LYS:HB2	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:B:323:THR:HA	1:B:326:MET:CE	2.40	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:F:83:GLU:HG2	2:F:1126:HOH:O	2.09	0.51
1:B:101:HIS:HD2	2:B:855:HOH:O	1.92	0.51
1:E:239:TYR:OH	1:E:261:GLU:OE1	2.21	0.51
1:D:163:THR:HG22	1:D:164:SER:H	1.71	0.51
1:F:327:ASP:OD1	1:F:329:THR:OG1	2.27	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:D:210:PHE:CE2	1:D:297:ILE:HG13	2.46	0.50
1:B:323:THR:HA	1:B:326:MET:HE2	1.94	0.50
1:B:100:PHE:HA	1:B:103:PHE:CD2	2.47	0.50
1:B:297:ILE:HG21	1:B:342:MET:HE3	1.92	0.50
1:E:190:SER:O	1:E:191:GLU:HB2	2.12	0.50
1:F:241:LYS:C	1:F:242:LYS:HD2	2.32	0.50
1:E:53:SER:OG	1:E:54:PHE:N	2.45	0.49
1:D:327:ASP:HB2	1:E:325:MET:O	2.12	0.49
1:A:311:LYS:HZ2	1:A:311:LYS:HB2	1.77	0.49
1:E:100:PHE:HA	1:E:103:PHE:CD2	2.47	0.49
1:A:120:GLN:HB2	2:A:1014:HOH:O	2.12	0.49
1:B:356:SER:O	1:B:360:ARG:HG3	2.11	0.49
1:D:308:GLN:HE22	1:D:315:LYS:NZ	2.11	0.49
1:B:320:GLN:H	1:B:320:GLN:CD	2.15	0.49
1:A:100:PHE:HA	1:A:103:PHE:CD2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:324:LEU:CD1	1:D:326:MET:HB2	2.43	0.49
1:A:85:ASP:HB3	1:A:88:ILE:HD12	1.94	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: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:B:80:ASP:OD1	2:B:884:HOH:O	2.20	0.47
1:D:324:LEU:CD1	1:D:326:MET:O	2.62	0.47
1:A:153:GLY:HA3	1:A:174:TYR:CG	2.49	0.47
1:C:348:ARG:NH1	1:C:348:ARG:HG3	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:N	1:B:315:LYS:HD3	2.15	0.46
1:F:51:SER:O	1:F:52:ARG:C	2.53	0.46
1:F:77:ARG:HD2	1:F:77:ARG:HA	1.76	0.46
1:D:166:GLN:CD	1:D:166:GLN:H	2.19	0.46
1:E:72:PHE:CZ	1:E:76:LEU:HD11	2.52	0.45
1:F:327:ASP:C	1:F:327:ASP:OD1	2.55	0.45
1:F:88:ILE:HG21	1:F:93:LYS:HG3	1.96	0.45
1:F:75:VAL:HG11	1:F:104:LEU:HD21	1.97	0.45
1:F:308:GLN:HA	1:F:311:LYS:HD3	1.99	0.45
1:D:316:ILE:H	1:D:316:ILE:HG13	1.57	0.45
1:F:54:PHE:CE1	1:F:57:VAL:CG2	2.97	0.45
1:B:53:SER:HB2	2:B:1249:HOH:O	2.16	0.45
1:F:368:THR:O	1:F:369:GLN:C	2.56	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:D:210:PHE:HE2	1:D:297:ILE:HG13	1.83	0.43
1:F:140:GLN:HG2	2:F:954:HOH:O	2.16	0.43
1:C:224:GLN:NE2	1:C:244:GLY:HA2	2.33	0.43
1:E:57:VAL:CG1	1:E:288:PHE:HA	2.47	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:D:224:GLN:HG2	2:D:879:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:LEU:HD21	1:B:303:CYS:O	2.19	0.42
1:F:140:GLN:HG3	2:F:954:HOH:O	2.14	0.42
1:F:121:VAL:HG23	1:F:128:ILE:CD1	2.47	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:C:326:MET:HB3	1:C:326:MET:HE3	1.72	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:C:292:PRO:HA	1:C:295:MET:HE2	2.02	0.42
1:B:297:ILE:HD13	1:B:338:ILE:HA	2.02	0.42
1:D:326:MET:HA	1:F:327:ASP:HB2	2.01	0.42
1:D:83:GLU:HB2	1:D:154:MET:HE3	1.99	0.42
1:E:314:VAL:HA	1:E:315:LYS:HE3	2.02	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:A:252:ILE:HD11	1:A:307:GLN:HB2	2.02	0.41
1:B:291:ILE:HD11	1:C:326:MET:HE3	2.02	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:B:297:ILE:H	1:B:297:ILE:HG13	1.67	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:F:262:LEU:O	1:F:265:ASN:HB3	2.21	0.41
1:C:246:PHE:HE2	1:C:258:CYS:HG	1.68	0.41
1:E:308:GLN:HB3	1:E:314:VAL:HG22	2.02	0.41
1:D:110:ARG:HD3	1:D:112:MET:SD	2.61	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:F:89:SER:HB3	1:F:92:LYS:HE3	2.03	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: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:F:369:GLN:O	1:F:369:GLN:CG	2.69	0.41
1:F:306:ASN:OD1	1:F:308:GLN:N	2.52	0.41
1:E:174:TYR:HA	1:E:178:LEU:HD12	2.04	0.41
1:D:215:ASN:OD1	1:D:218:ARG:NH2	2.54	0.41
1:F:100:PHE:HA	1:F:103:PHE:CD2	2.55	0.41
1:F:213:LYS:HE2	1:F:265:ASN:OD1	2.22	0.40
1:C:236:TRP:CE2	1:C:243:LEU:HB2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:125:PHE:N	1:F:126:PRO:CD	2.84	0.40
1:F:54:PHE:CE1	1:F:292:PRO:HG3	2.56	0.40
1:B:322:VAL:O	1:B:326:MET:HE2	2.22	0.40
1:D:348:ARG:CG	1:D:348:ARG:NH1	2.82	0.40
1:C:353:ASP:HB3	1:C:356:SER:HB3	2.03	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 (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	319/343 (93%)	313 (98%)	6 (2%)	0	100	100
1	B	331/343 (96%)	321 (97%)	8 (2%)	2 (1%)	30	18
1	C	330/343 (96%)	321 (97%)	8 (2%)	1 (0%)	46	36
1	D	326/343 (95%)	314 (96%)	12 (4%)	0	100	100
1	E	325/343 (95%)	314 (97%)	10 (3%)	1 (0%)	46	36
1	F	320/343 (93%)	304 (95%)	16 (5%)	0	100	100
All	All	1951/2058 (95%)	1887 (97%)	60 (3%)	4 (0%)	52	43

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 (i)

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%)	279 (97%)	9 (3%)	47	39
1	B	296/305 (97%)	283 (96%)	13 (4%)	35	26
1	C	298/305 (98%)	286 (96%)	12 (4%)	38	29
1	D	295/305 (97%)	275 (93%)	20 (7%)	20	11
1	E	293/305 (96%)	283 (97%)	10 (3%)	44	36
1	F	290/305 (95%)	271 (93%)	19 (7%)	21	11
All	All	1760/1830 (96%)	1677 (95%)	83 (5%)	32	23

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LEU
1	A	37	SER
1	A	38	SER
1	A	159	ASP
1	A	199	GLU
1	A	225	GLN
1	A	311	LYS
1	A	327	ASP
1	A	358	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

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Mol	Chain	Res	Type
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	311	LYS
1	C	348	ARG
1	C	351	ASP
1	C	369	GLN
1	D	76	LEU
1	D	77	ARG
1	D	84	ASP
1	D	87	THR
1	D	91	GLU
1	D	96	LEU
1	D	102	SER
1	D	115	LYS
1	D	117	LYS
1	D	158	LEU
1	D	194	ASP
1	D	203	ARG
1	D	242	LYS
1	D	311	LYS
1	D	315	LYS
1	D	318	LYS
1	D	323	THR
1	D	348	ARG
1	D	358	LYS
1	D	361	GLN
1	E	54	PHE
1	E	77	ARG
1	E	83	GLU
1	E	91	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

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Mol	Chain	Res	Type
1	F	51	SER
1	F	53	SER
1	F	91	GLU
1	F	92	LYS
1	F	96	LEU
1	F	113	GLU
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	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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	225	GLN
1	A	283	GLN
1	A	307	GLN
1	B	59	GLN
1	B	101	HIS
1	B	140	GLN
1	B	224	GLN
1	B	308	GLN
1	B	340	GLN
1	C	49	GLN
1	C	59	GLN
1	C	101	HIS
1	C	224	GLN
1	C	293	GLN
1	C	307	GLN
1	D	49	GLN
1	D	59	GLN
1	D	98	HIS
1	D	140	GLN

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Mol	Chain	Res	Type
1	D	173	HIS
1	D	306	ASN
1	D	308	GLN
1	D	340	GLN
1	E	49	GLN
1	E	140	GLN
1	E	282	ASN
1	E	308	GLN
1	E	361	GLN
1	F	49	GLN
1	F	98	HIS
1	F	106	GLN
1	F	120	GLN
1	F	140	GLN
1	F	283	GLN
1	F	308	GLN
1	F	340	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

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, 95^{th} 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%)	0.04	4 (1%) 81 84	24, 35, 60, 75	0
1	B	333/343 (97%)	0.32	24 (7%) 18 22	29, 41, 78, 98	0
1	C	334/343 (97%)	0.42	23 (6%) 20 23	25, 39, 85, 108	0
1	D	330/343 (96%)	0.54	32 (9%) 10 11	38, 59, 98, 116	0
1	E	329/343 (95%)	0.57	38 (11%) 6 7	28, 47, 89, 104	0
1	F	324/343 (94%)	0.97	69 (21%) 1 1	34, 72, 117, 136	0
All	All	1973/2058 (95%)	0.48	190 (9%) 10 11	24, 48, 97, 136	0

All (190) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	324	LEU	10.5
1	B	319	GLY	8.9
1	C	313	ALA	7.8
1	F	250	GLU	7.4
1	C	315	LYS	7.1
1	E	241	LYS	6.4
1	D	313	ALA	6.3
1	F	323	THR	6.2
1	F	230	PHE	6.1
1	C	314	VAL	5.9
1	B	318	LYS	5.8
1	F	243	LEU	5.8
1	F	229	GLU	5.7
1	D	115	LYS	5.6
1	E	324	LEU	5.6
1	F	241	LYS	5.6
1	E	52	ARG	5.6
1	E	313	ALA	5.5
1	B	317	ARG	5.5

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Mol	Chain	Res	Type	RSRZ
1	D	317	ARG	5.4
1	C	312	GLY	5.3
1	D	117	LYS	5.2
1	F	244	GLY	5.2
1	B	316	ILE	5.1
1	E	211	LEU	5.1
1	F	347	HIS	5.0
1	D	325	MET	4.9
1	F	117	LYS	4.9
1	E	242	LYS	4.8
1	F	162	VAL	4.8
1	A	312	GLY	4.8
1	F	167	GLU	4.7
1	E	323	THR	4.6
1	C	316	ILE	4.6
1	E	228	ARG	4.5
1	F	159	ASP	4.4
1	E	225	GLN	4.4
1	F	325	MET	4.2
1	F	247	ALA	4.1
1	F	160	LYS	4.1
1	E	226	GLY	4.0
1	F	225	GLN	4.0
1	F	239	TYR	3.9
1	F	252	ILE	3.9
1	F	158	LEU	3.9
1	F	222	GLU	3.9
1	A	313	ALA	3.9
1	F	88	ILE	3.8
1	F	310	PHE	3.8
1	E	351	ASP	3.8
1	F	251	ASN	3.8
1	B	225	GLN	3.8
1	D	318	LYS	3.7
1	C	317	ARG	3.7
1	D	161	HIS	3.7
1	B	320	GLN	3.7
1	E	37	SER	3.6
1	C	52	ARG	3.6
1	D	37	SER	3.6
1	F	85	ASP	3.5
1	D	159	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	179	VAL	3.5
1	F	113	GLU	3.4
1	E	263	ILE	3.4
1	E	214	THR	3.4
1	F	235	VAL	3.4
1	E	224	GLN	3.4
1	D	119	ARG	3.4
1	F	170	LYS	3.3
1	F	242	LYS	3.3
1	F	249	PRO	3.3
1	B	313	ALA	3.3
1	D	322	VAL	3.3
1	C	368	THR	3.3
1	E	352	SER	3.3
1	F	246	PHE	3.3
1	E	245	ASP	3.2
1	B	37	SER	3.2
1	C	242	LYS	3.2
1	A	325	MET	3.2
1	F	53	SER	3.1
1	F	161	HIS	3.1
1	D	228	ARG	3.1
1	E	347	HIS	3.1
1	E	349	ILE	3.0
1	F	86	MET	3.0
1	D	324	LEU	3.0
1	F	256	VAL	3.0
1	E	227	GLY	3.0
1	D	107	PRO	3.0
1	F	121	VAL	3.0
1	F	245	ASP	3.0
1	B	315	LYS	3.0
1	D	316	ILE	2.9
1	B	183	LEU	2.9
1	E	221	LEU	2.9
1	D	120	GLN	2.9
1	F	254	LEU	2.9
1	D	86	MET	2.9
1	F	105	TYR	2.9
1	E	243	LEU	2.9
1	E	240	VAL	2.9
1	A	249	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	309	VAL	2.9
1	E	161	HIS	2.8
1	D	226	GLY	2.8
1	F	91	GLU	2.8
1	E	251	ASN	2.8
1	F	248	LYS	2.8
1	B	236	TRP	2.8
1	F	99	ASN	2.8
1	E	159	ASP	2.8
1	D	312	GLY	2.8
1	E	322	VAL	2.8
1	C	159	ASP	2.7
1	F	115	LYS	2.7
1	F	116	GLU	2.7
1	D	130	LEU	2.7
1	C	347	HIS	2.7
1	F	37	SER	2.7
1	C	239	TYR	2.7
1	F	220	TYR	2.7
1	D	183	LEU	2.6
1	D	281	ARG	2.6
1	C	241	LYS	2.6
1	F	165	GLU	2.6
1	F	240	VAL	2.6
1	D	87	THR	2.6
1	D	314	VAL	2.5
1	F	54	PHE	2.5
1	E	87	THR	2.5
1	D	137	GLU	2.5
1	E	244	GLY	2.4
1	F	114	SER	2.4
1	F	120	GLN	2.4
1	D	196	LEU	2.4
1	F	221	LEU	2.4
1	F	228	ARG	2.4
1	F	322	VAL	2.4
1	D	189	ALA	2.4
1	E	117	LYS	2.4
1	E	239	TYR	2.4
1	B	226	GLY	2.4
1	B	227	GLY	2.4
1	B	228	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	76	LEU	2.4
1	F	157	PHE	2.4
1	F	152	ILE	2.3
1	E	315	LYS	2.3
1	D	104	LEU	2.3
1	F	89	SER	2.3
1	E	236	TRP	2.3
1	F	226	GLY	2.3
1	D	118	ASP	2.3
1	B	52	ARG	2.3
1	B	143	ILE	2.3
1	D	90	VAL	2.2
1	C	34	ASP	2.2
1	C	115	LYS	2.2
1	C	210	PHE	2.2
1	E	210	PHE	2.2
1	C	369	GLN	2.2
1	C	323	THR	2.2
1	B	182	GLY	2.2
1	C	161	HIS	2.2
1	B	324	LEU	2.2
1	F	87	THR	2.2
1	B	297	ILE	2.2
1	F	52	ARG	2.2
1	D	369	GLN	2.2
1	F	112	MET	2.2
1	F	231	TRP	2.2
1	B	161	HIS	2.2
1	F	307	GLN	2.2
1	F	127	THR	2.1
1	E	314	VAL	2.1
1	F	166	GLN	2.1
1	E	217	ILE	2.1
1	B	159	ASP	2.1
1	D	323	THR	2.1
1	E	222	GLU	2.1
1	C	289	CYS	2.1
1	F	327	ASP	2.1
1	F	236	TRP	2.1
1	C	238	ARG	2.1
1	B	249	PRO	2.1
1	B	240	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	297	ILE	2.0
1	C	324	LEU	2.0
1	E	234	GLU	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 carbohydrates 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.