Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 05:08 am BST

PDB ID	:	5NDY
Title	:	crystal structure of variants
Authors	:	Linde, M.; Rajendran, C.; Babinger, P.; Sterner, R.
Deposited on	:	2017-03-09
Resolution	:	1.95 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 following versions of software and data (see references ⓘ) were used in the production of this report:

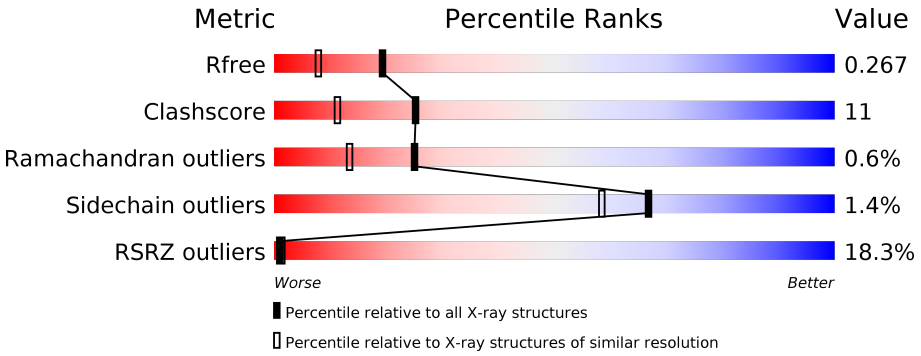
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 1.95 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}	130704	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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 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 <=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	256	10% 84% 10% • 5%
1	B	256	12% 81% 13% • 5%
1	C	256	11% 83% 11% 5%
1	D	256	27% 71% 20% • 8%
1	E	256	23% 71% 20% • 7%
1	F	256	21% 73% 20% • 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11331 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 Geranylgeranylglyceryl phosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	243	Total	C	N	O	S	0	0	0
			1825	1154	308	352	11			
1	B	244	Total	C	N	O	S	0	0	0
			1824	1153	308	353	10			
1	C	242	Total	C	N	O	S	0	0	0
			1813	1145	306	351	11			
1	D	236	Total	C	N	O	S	0	0	0
			1750	1106	296	339	9			
1	E	238	Total	C	N	O	S	0	0	0
			1768	1117	295	346	10			
1	F	241	Total	C	N	O	S	0	0	0
			1802	1137	304	350	11			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP O26652
A	2	PHE	-	expression tag	UNP O26652
A	3	LYS	-	expression tag	UNP O26652
A	162	GLU	ALA	conflict	UNP O26652
A	249	LEU	-	expression tag	UNP O26652
A	250	GLU	-	expression tag	UNP O26652
A	251	HIS	-	expression tag	UNP O26652
A	252	HIS	-	expression tag	UNP O26652
A	253	HIS	-	expression tag	UNP O26652
A	254	HIS	-	expression tag	UNP O26652
A	255	HIS	-	expression tag	UNP O26652
A	256	HIS	-	expression tag	UNP O26652
B	1	MET	-	initiating methionine	UNP O26652
B	2	PHE	-	expression tag	UNP O26652
B	3	LYS	-	expression tag	UNP O26652
B	162	GLU	ALA	conflict	UNP O26652
B	249	LEU	-	expression tag	UNP O26652

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Chain	Residue	Modelled	Actual	Comment	Reference
B	250	GLU	-	expression tag	UNP O26652
B	251	HIS	-	expression tag	UNP O26652
B	252	HIS	-	expression tag	UNP O26652
B	253	HIS	-	expression tag	UNP O26652
B	254	HIS	-	expression tag	UNP O26652
B	255	HIS	-	expression tag	UNP O26652
B	256	HIS	-	expression tag	UNP O26652
C	1	MET	-	initiating methionine	UNP O26652
C	2	PHE	-	expression tag	UNP O26652
C	3	LYS	-	expression tag	UNP O26652
C	162	GLU	ALA	conflict	UNP O26652
C	249	LEU	-	expression tag	UNP O26652
C	250	GLU	-	expression tag	UNP O26652
C	251	HIS	-	expression tag	UNP O26652
C	252	HIS	-	expression tag	UNP O26652
C	253	HIS	-	expression tag	UNP O26652
C	254	HIS	-	expression tag	UNP O26652
C	255	HIS	-	expression tag	UNP O26652
C	256	HIS	-	expression tag	UNP O26652
D	1	MET	-	initiating methionine	UNP O26652
D	2	PHE	-	expression tag	UNP O26652
D	3	LYS	-	expression tag	UNP O26652
D	162	GLU	ALA	conflict	UNP O26652
D	249	LEU	-	expression tag	UNP O26652
D	250	GLU	-	expression tag	UNP O26652
D	251	HIS	-	expression tag	UNP O26652
D	252	HIS	-	expression tag	UNP O26652
D	253	HIS	-	expression tag	UNP O26652
D	254	HIS	-	expression tag	UNP O26652
D	255	HIS	-	expression tag	UNP O26652
D	256	HIS	-	expression tag	UNP O26652
E	1	MET	-	initiating methionine	UNP O26652
E	2	PHE	-	expression tag	UNP O26652
E	3	LYS	-	expression tag	UNP O26652
E	162	GLU	ALA	conflict	UNP O26652
E	249	LEU	-	expression tag	UNP O26652
E	250	GLU	-	expression tag	UNP O26652
E	251	HIS	-	expression tag	UNP O26652
E	252	HIS	-	expression tag	UNP O26652
E	253	HIS	-	expression tag	UNP O26652
E	254	HIS	-	expression tag	UNP O26652
E	255	HIS	-	expression tag	UNP O26652

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Chain	Residue	Modelled	Actual	Comment	Reference
E	256	HIS	-	expression tag	UNP O26652
F	1	MET	-	initiating methionine	UNP O26652
F	2	PHE	-	expression tag	UNP O26652
F	3	LYS	-	expression tag	UNP O26652
F	162	GLU	ALA	conflict	UNP O26652
F	249	LEU	-	expression tag	UNP O26652
F	250	GLU	-	expression tag	UNP O26652
F	251	HIS	-	expression tag	UNP O26652
F	252	HIS	-	expression tag	UNP O26652
F	253	HIS	-	expression tag	UNP O26652
F	254	HIS	-	expression tag	UNP O26652
F	255	HIS	-	expression tag	UNP O26652
F	256	HIS	-	expression tag	UNP O26652

- Molecule 2 is water.

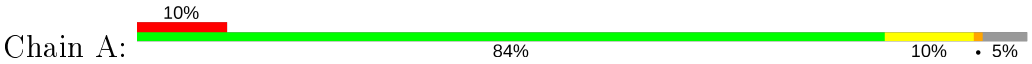
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	145	Total O 145 145	0	0
2	B	132	Total O 132 132	0	0
2	C	122	Total O 122 122	0	0
2	D	45	Total O 45 45	0	0
2	E	60	Total O 60 60	0	0
2	F	45	Total O 45 45	0	0

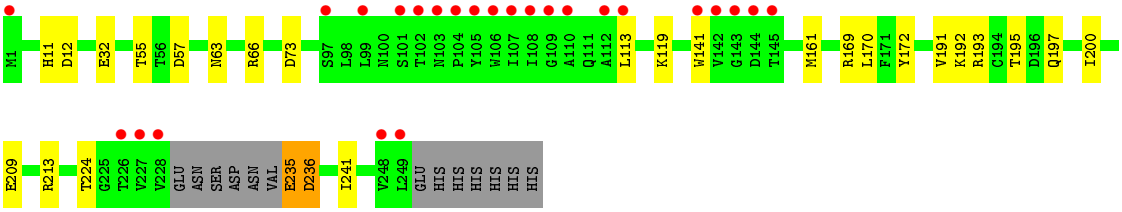
3 Residue-property plots (i)

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

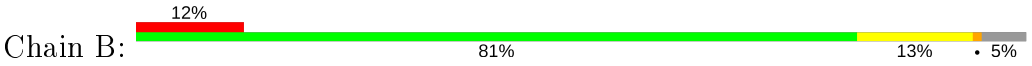
Chain A:

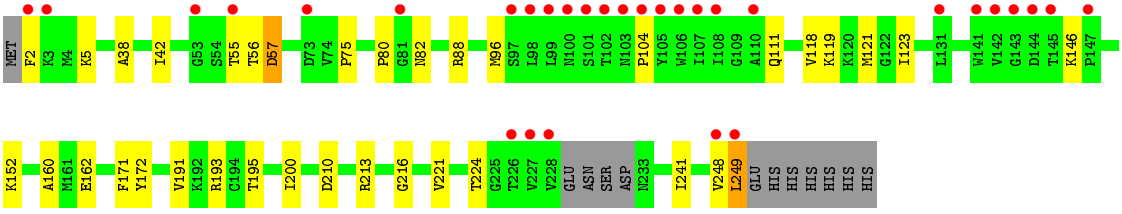




- Molecule 1: Geranylgeranylglyceryl phosphate synthase

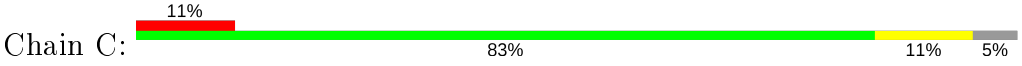
Chain B:

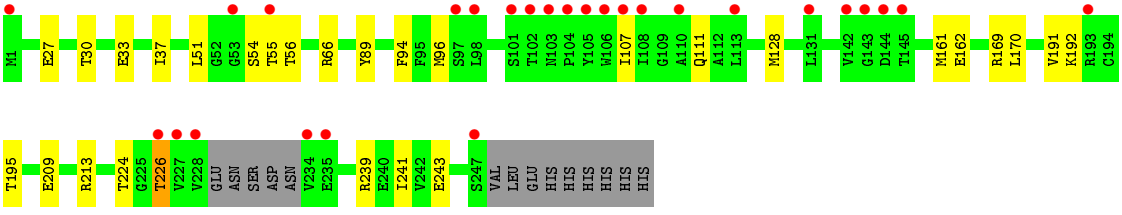




- Molecule 1: Geranylgeranylglyceryl phosphate synthase

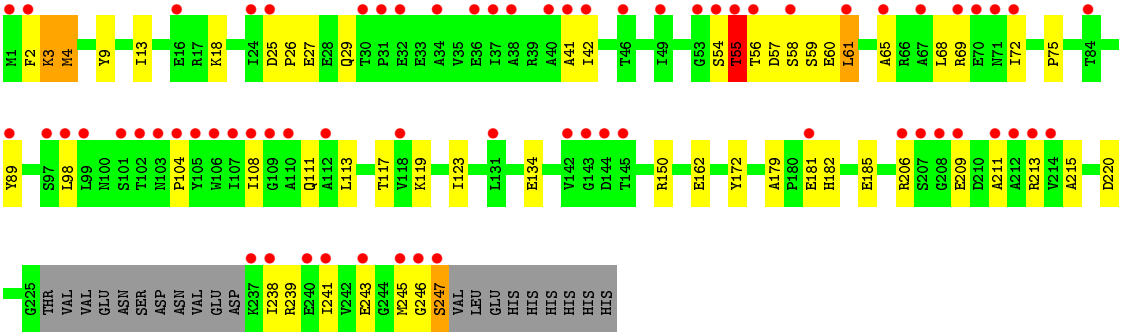
Chain C:





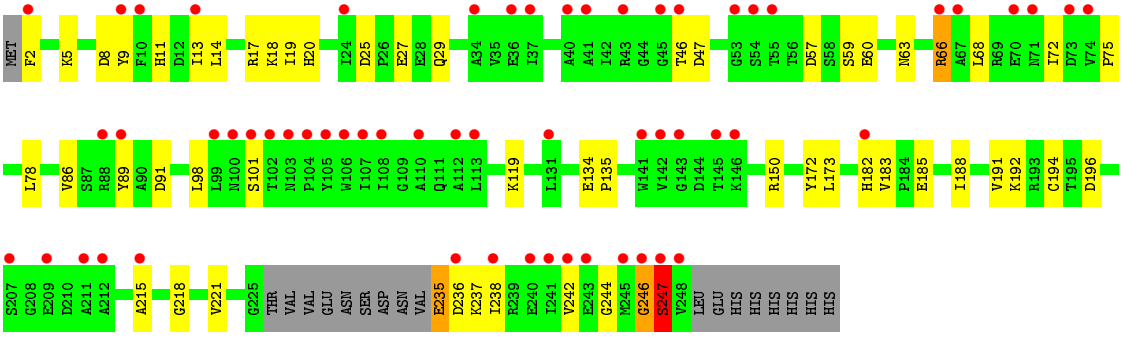
- Molecule 1: Geranylgeranylglyceryl phosphate synthase

Chain D:



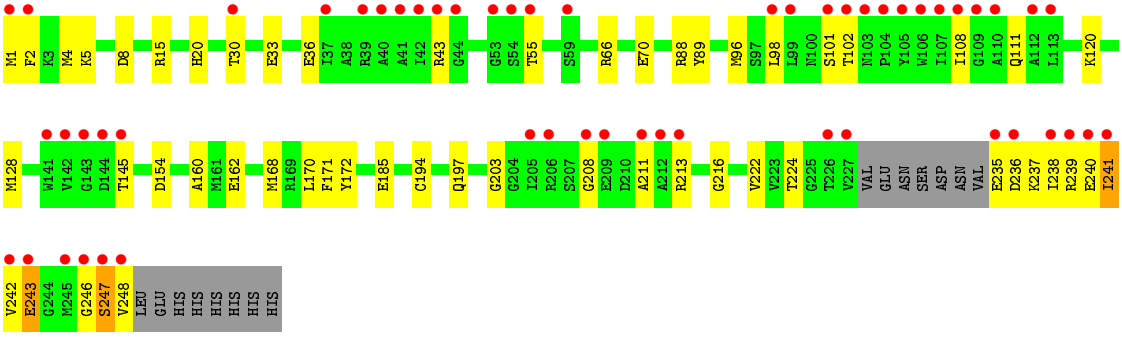
• Molecule 1: Geranylgeranylglyceryl phosphate synthase

Chain E:



• Molecule 1: Geranylgeranylglyceryl phosphate synthase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	142.54Å 147.66Å 90.35Å 90.00° 108.99° 90.00°	Depositor
Resolution (Å)	49.77 – 1.95 49.77 – 1.95	Depositor EDS
% Data completeness (in resolution range)	97.4 (49.77-1.95) 97.5 (49.77-1.95)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.01 (at 1.95Å)	Xtriage
Refinement program	PHENIX (1.10pre_2119: ???)	Depositor
R, R_{free}	0.218 , 0.262 0.235 , 0.267	Depositor DCC
R_{free} test set	6259 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	37.0	Xtriage
Anisotropy	0.485	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 46.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11331	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% 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, 0.333 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	0.49	0/1855	0.63	1/2513 (0.0%)
1	B	0.47	0/1854	0.57	0/2514
1	C	0.46	0/1843	0.60	0/2498
1	D	0.40	0/1780	0.65	5/2415 (0.2%)
1	E	0.40	0/1798	0.56	1/2440 (0.0%)
1	F	0.41	0/1832	0.60	1/2484 (0.0%)
All	All	0.44	0/10962	0.60	8/14864 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	61	LEU	CB-CG-CD1	-8.49	96.56	111.00
1	D	61	LEU	CB-CG-CD2	7.74	124.16	111.00
1	F	241	ILE	CG1-CB-CG2	-5.77	98.72	111.40
1	E	246	GLY	N-CA-C	-5.62	99.05	113.10
1	A	235	GLU	N-CA-C	-5.52	96.11	111.00
1	D	56	THR	N-CA-C	5.38	125.53	111.00
1	D	61	LEU	CA-CB-CG	-5.04	103.72	115.30
1	D	3	LYS	N-CA-C	-5.02	97.45	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1825	0	1834	22	0
1	B	1824	0	1821	31	0
1	C	1813	0	1812	27	0
1	D	1750	0	1727	59	0
1	E	1768	0	1742	49	0
1	F	1802	0	1792	56	0
2	A	145	0	0	7	0
2	B	132	0	0	2	0
2	C	122	0	0	5	0
2	D	45	0	0	3	0
2	E	60	0	0	8	0
2	F	45	0	0	4	0
All	All	11331	0	10728	229	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 11.

All (229) 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:E:2:PHE:HE2	1:E:75:PRO:HD3	1.06	1.14
1:F:238:ILE:O	1:F:242:VAL:HG23	1.46	1.14
1:D:54:SER:HA	1:D:55:THR:OG1	1.44	1.14
1:E:2:PHE:CE2	1:E:75:PRO:HD3	1.83	1.14
1:F:211:ALA:HB2	1:F:241:ILE:HD12	1.17	1.11
1:F:211:ALA:CB	1:F:241:ILE:HD12	1.93	0.98
1:C:37:ILE:CG2	1:C:226:THR:HG21	1.95	0.96
1:D:26:PRO:HG3	1:D:61:LEU:HD11	1.48	0.94
1:C:37:ILE:HG21	1:C:226:THR:HG21	1.51	0.93
1:D:123:ILE:O	2:D:301:HOH:O	1.88	0.91
1:B:55:THR:O	2:B:301:HOH:O	1.89	0.90
1:F:246:GLY:O	1:F:247:SER:OG	1.91	0.87
1:E:2:PHE:CE2	1:E:75:PRO:CD	2.59	0.86
1:F:203:GLY:O	2:F:301:HOH:O	1.95	0.85
1:D:54:SER:CA	1:D:55:THR:OG1	2.26	0.83
1:E:135:PRO:O	2:E:302:HOH:O	1.95	0.83
1:F:43:ARG:O	1:F:239:ARG:NH2	2.12	0.82
1:A:193:ARG:NH1	2:A:301:HOH:O	2.06	0.80
1:B:119:LYS:NZ	1:F:194:CYS:O	2.14	0.80
1:D:150:ARG:NH2	1:D:182:HIS:O	2.15	0.79
1:A:119:LYS:NZ	1:E:194:CYS:O	2.16	0.79
1:F:239:ARG:O	1:F:243:GLU:N	2.13	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:9:TYR:OH	2:E:301:HOH:O	1.93	0.78
1:D:54:SER:HA	1:D:55:THR:CB	2.14	0.77
1:E:66:ARG:HD3	1:E:89:TYR:HE1	1.50	0.76
1:E:66:ARG:HD3	1:E:89:TYR:CE1	2.21	0.76
1:F:4:MET:HE3	1:F:5:LYS:HB2	1.66	0.75
1:E:25:ASP:O	1:E:29:GLN:NE2	2.18	0.74
1:E:238:ILE:HG22	1:E:242:VAL:HG23	1.68	0.73
1:C:56:THR:OG1	2:C:301:HOH:O	2.05	0.73
1:F:66:ARG:HG3	1:F:89:TYR:CE2	2.23	0.73
1:B:248:VAL:HG13	1:B:249:LEU:HD22	1.73	0.71
1:F:154:ASP:O	2:F:302:HOH:O	2.08	0.70
1:B:55:THR:HG21	1:D:113:LEU:HD13	1.74	0.69
1:E:134:GLU:HG2	1:E:150:ARG:HG3	1.73	0.69
1:D:181:GLU:N	1:D:181:GLU:OE2	2.26	0.69
1:E:150:ARG:NH2	1:E:182:HIS:O	2.21	0.69
1:D:206:ARG:HH11	1:D:206:ARG:HG3	1.58	0.69
1:D:54:SER:CA	1:D:55:THR:CB	2.70	0.68
1:D:134:GLU:HG2	1:D:150:ARG:HG3	1.74	0.68
1:D:54:SER:HA	1:D:55:THR:HG1	1.58	0.68
1:D:134:GLU:OE2	2:D:302:HOH:O	2.12	0.68
1:F:120:LYS:NZ	2:F:303:HOH:O	2.16	0.67
1:F:222:VAL:HG11	1:F:241:ILE:HD11	1.76	0.67
1:E:196:ASP:OD2	2:E:303:HOH:O	2.13	0.67
1:A:73:ASP:OD2	2:A:302:HOH:O	2.12	0.66
1:C:30:THR:HG23	1:C:33:GLU:H	1.60	0.65
1:E:47:ASP:O	2:E:301:HOH:O	2.15	0.65
1:D:239:ARG:O	1:D:243:GLU:HG2	1.97	0.64
1:D:42:ILE:HD12	1:D:72:ILE:HD11	1.78	0.64
1:A:113:LEU:HB3	1:F:55:THR:HG21	1.78	0.64
1:E:91:ASP:O	2:E:304:HOH:O	2.15	0.64
1:C:37:ILE:HG23	1:C:226:THR:HG21	1.78	0.64
1:F:4:MET:CE	1:F:5:LYS:HB2	2.28	0.64
1:D:42:ILE:CD1	1:D:72:ILE:HD11	2.27	0.63
1:B:248:VAL:CG1	1:B:249:LEU:HD22	2.28	0.63
1:E:235:GLU:O	1:E:237:LYS:N	2.29	0.62
1:C:27:GLU:HB3	1:C:56:THR:HG21	1.81	0.62
1:B:249:LEU:HD13	1:B:249:LEU:N	2.13	0.62
1:A:235:GLU:HG2	1:A:236:ASP:H	1.64	0.61
1:F:20:HIS:HE2	1:F:224:THR:HG1	1.46	0.61
1:B:210:ASP:OD1	1:B:213:ARG:NH2	2.34	0.60
1:B:249:LEU:H	1:B:249:LEU:HD22	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:54:SER:CB	1:D:55:THR:HB	2.32	0.60
1:D:2:PHE:CZ	1:D:75:PRO:HG3	2.36	0.60
1:D:57:ASP:OD1	1:D:58:SER:N	2.34	0.60
1:B:249:LEU:HD13	1:B:249:LEU:H	1.67	0.60
1:D:54:SER:HB2	1:D:55:THR:C	2.22	0.60
1:E:119:LYS:NZ	2:E:308:HOH:O	2.35	0.59
1:B:224:THR:HG21	1:B:241:ILE:HD13	1.84	0.59
1:B:118:VAL:HG13	1:B:123:ILE:HG23	1.85	0.59
1:F:211:ALA:HB2	1:F:241:ILE:CD1	2.12	0.59
1:E:5:LYS:HE3	1:E:8:ASP:OD2	2.04	0.58
1:F:30:THR:HG22	1:F:33:GLU:HG3	1.85	0.58
1:B:57:ASP:HB2	1:D:117:THR:HG21	1.86	0.58
1:A:11:HIS:ND1	2:A:306:HOH:O	2.31	0.58
1:C:192:LYS:HE2	2:C:331:HOH:O	2.04	0.58
1:E:14:LEU:HA	1:E:17:ARG:O	2.04	0.57
1:A:57:ASP:OD2	2:F:303:HOH:O	2.17	0.57
1:D:26:PRO:HG3	1:D:61:LEU:CD1	2.29	0.57
1:E:235:GLU:OE2	1:E:235:GLU:N	2.38	0.56
1:F:66:ARG:HG3	1:F:89:TYR:CD2	2.40	0.56
1:E:19:ILE:HB	1:E:221:VAL:HG22	1.87	0.56
1:D:26:PRO:CG	1:D:61:LEU:HD11	2.30	0.56
1:E:238:ILE:HG22	1:E:242:VAL:CG2	2.33	0.56
1:B:55:THR:HG23	1:B:82:ASN:HB2	1.88	0.56
1:D:185:GLU:OE2	1:D:213:ARG:HB3	2.05	0.55
1:C:111:GLN:HB2	1:D:162:GLU:OE2	2.05	0.55
1:C:224:THR:HG21	1:C:241:ILE:HD13	1.87	0.55
1:D:246:GLY:HA2	1:D:247:SER:C	2.26	0.55
1:D:179:ALA:O	1:D:206:ARG:NH2	2.40	0.55
1:D:25:ASP:O	1:D:29:GLN:NE2	2.36	0.55
1:A:191:VAL:O	1:A:195:THR:HG22	2.07	0.55
1:B:88:ARG:HG3	1:B:121:MET:HG2	1.88	0.55
1:E:244:GLY:C	1:E:246:GLY:H	2.09	0.54
1:E:66:ARG:HA	1:E:89:TYR:CE1	2.43	0.54
1:C:239:ARG:O	1:C:243:GLU:HG3	2.08	0.54
1:F:216:GLY:HA2	1:F:248:VAL:CG1	2.38	0.54
1:A:193:ARG:HD2	2:A:301:HOH:O	2.08	0.53
1:D:220:ASP:OD1	2:D:303:HOH:O	2.19	0.53
1:F:168:MET:O	1:F:197:GLN:NE2	2.41	0.53
1:E:2:PHE:HZ	1:E:9:TYR:CD2	2.27	0.53
1:F:235:GLU:C	1:F:237:LYS:H	2.12	0.53
1:F:160:ALA:HA	1:F:171:PHE:CE1	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:240:GLU:HA	1:F:243:GLU:HB2	1.91	0.52
1:F:4:MET:CE	1:F:5:LYS:H	2.22	0.52
1:B:111:GLN:HB2	1:F:162:GLU:OE2	2.09	0.52
1:F:20:HIS:NE2	1:F:224:THR:OG1	2.37	0.52
1:A:63:ASN:OD1	1:A:66:ARG:NH2	2.42	0.52
1:C:94:PHE:HB3	1:C:96:MET:HE3	1.92	0.52
1:A:235:GLU:CG	1:A:236:ASP:H	2.20	0.51
1:C:128:MET:HE2	1:C:170:LEU:CB	2.40	0.51
1:D:246:GLY:N	1:D:247:SER:HB2	2.26	0.51
1:E:185:GLU:HB2	2:E:321:HOH:O	2.10	0.51
1:D:54:SER:HB2	1:D:55:THR:HB	1.92	0.51
1:B:80:PRO:HD2	1:B:96:MET:HE3	1.93	0.51
1:F:30:THR:CG2	1:F:33:GLU:HG3	2.41	0.51
1:E:20:HIS:O	1:E:47:ASP:HB2	2.11	0.51
1:B:200:ILE:HG12	1:B:221:VAL:HB	1.93	0.50
1:C:209:GLU:O	1:C:213:ARG:HG2	2.12	0.50
1:E:78:LEU:HD13	1:E:86:VAL:HA	1.94	0.50
1:F:33:GLU:O	1:F:36:GLU:HB2	2.12	0.50
1:E:183:VAL:HB	1:E:188:ILE:HD11	1.92	0.50
1:F:66:ARG:NH1	1:F:70:GLU:OE2	2.45	0.49
1:A:192:LYS:HE2	2:A:354:HOH:O	2.11	0.49
1:B:38:ALA:O	1:B:42:ILE:HG12	2.11	0.49
1:E:66:ARG:HA	1:E:89:TYR:CD1	2.47	0.49
1:A:12:ASP:OD1	2:A:303:HOH:O	2.19	0.48
1:D:68:LEU:O	1:D:72:ILE:HG22	2.13	0.48
1:E:235:GLU:C	1:E:237:LYS:H	2.13	0.48
1:D:150:ARG:CZ	1:D:181:GLU:HG2	2.43	0.48
1:C:161:MET:SD	1:D:119:LYS:HD2	2.53	0.48
1:C:128:MET:HE2	1:C:170:LEU:HB3	1.94	0.48
1:A:55:THR:O	1:A:55:THR:OG1	2.29	0.48
1:E:173:LEU:HD11	1:E:191:VAL:HG21	1.95	0.48
1:F:1:MET:SD	1:F:2:PHE:N	2.86	0.48
1:B:5:LYS:NZ	2:B:308:HOH:O	2.43	0.47
1:C:162:GLU:OE2	1:D:111:GLN:HB2	2.14	0.47
1:F:185:GLU:OE2	1:F:213:ARG:NH2	2.47	0.47
1:F:239:ARG:O	1:F:243:GLU:HB2	2.13	0.47
1:B:104:PRO:HG3	1:F:102:THR:O	2.15	0.47
1:D:61:LEU:N	1:D:61:LEU:HD12	2.28	0.47
1:E:68:LEU:O	1:E:72:ILE:HG12	2.15	0.47
1:D:206:ARG:CG	1:D:206:ARG:HH11	2.25	0.47
1:D:68:LEU:HD23	1:D:68:LEU:HA	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:241:ILE:HG22	1:D:245:MET:HE1	1.98	0.46
1:D:65:ALA:HB1	1:D:89:TYR:HB2	1.98	0.46
1:B:193:ARG:HG2	1:B:193:ARG:HH11	1.81	0.46
1:E:11:HIS:HE1	2:E:313:HOH:O	1.98	0.46
1:F:66:ARG:HD3	1:F:89:TYR:CZ	2.51	0.46
1:D:211:ALA:HB2	1:D:241:ILE:HG23	1.98	0.46
1:C:191:VAL:O	1:C:195:THR:HG22	2.16	0.45
1:F:30:THR:HG22	1:F:33:GLU:OE2	2.16	0.45
1:D:2:PHE:CD2	1:D:3:LYS:O	2.70	0.45
1:F:30:THR:N	1:F:33:GLU:OE2	2.36	0.45
1:A:170:LEU:HD23	1:A:200:ILE:HD11	1.99	0.45
1:D:246:GLY:CA	1:D:247:SER:HB2	2.47	0.45
1:A:32:GLU:HG3	2:A:343:HOH:O	2.17	0.45
1:D:9:TYR:CZ	1:D:13:ILE:HD11	2.52	0.44
1:F:238:ILE:HA	1:F:241:ILE:HG22	1.99	0.44
1:E:20:HIS:ND1	1:E:46:THR:OG1	2.41	0.44
1:B:216:GLY:HA2	1:B:248:VAL:HG11	1.98	0.44
1:F:128:MET:HE2	1:F:170:LEU:HB3	1.99	0.44
1:D:18:LYS:HD3	1:D:215:ALA:HB1	2.00	0.44
1:D:241:ILE:HG22	1:D:245:MET:CE	2.47	0.44
1:A:224:THR:HG21	1:A:241:ILE:HD13	1.98	0.44
1:C:66:ARG:HD3	1:C:89:TYR:CZ	2.53	0.44
1:E:238:ILE:CG2	1:E:242:VAL:HG23	2.44	0.44
1:E:27:GLU:HA	1:E:60:GLU:OE2	2.18	0.44
1:F:98:LEU:HG	1:F:101:SER:HB2	1.99	0.44
1:D:206:ARG:NH1	1:D:206:ARG:HG3	2.30	0.43
1:D:27:GLU:HG3	1:D:60:GLU:OE1	2.18	0.43
1:A:113:LEU:HD22	1:F:55:THR:HB	2.00	0.43
1:F:240:GLU:HA	1:F:243:GLU:CB	2.48	0.43
1:F:4:MET:HE3	1:F:8:ASP:HB2	1.99	0.43
1:D:54:SER:CB	1:D:55:THR:CB	2.96	0.43
1:B:160:ALA:HA	1:B:171:PHE:CE1	2.53	0.43
1:D:41:ALA:HA	1:D:238:ILE:HD13	2.01	0.43
1:E:2:PHE:HE2	1:E:75:PRO:CD	1.96	0.43
1:D:206:ARG:NH1	1:D:206:ARG:CG	2.81	0.43
1:F:246:GLY:O	1:F:247:SER:CB	2.66	0.43
1:B:191:VAL:O	1:B:195:THR:HG22	2.19	0.43
1:E:192:LYS:HE3	1:E:218:GLY:O	2.18	0.43
1:E:244:GLY:C	1:E:246:GLY:N	2.72	0.42
1:D:69:ARG:NH2	1:D:89:TYR:HD1	2.17	0.42
1:E:98:LEU:HG	1:E:101:SER:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:88:ARG:NH1	1:F:89:TYR:OH	2.53	0.42
1:B:152:LYS:HA	1:B:152:LYS:HD3	1.88	0.42
1:D:65:ALA:CB	1:D:89:TYR:HB2	2.49	0.42
1:D:3:LYS:O	1:D:4:MET:CB	2.68	0.42
1:D:57:ASP:OD2	1:D:59:SER:OG	2.37	0.42
1:E:134:GLU:CG	1:E:150:ARG:HG3	2.45	0.42
1:E:57:ASP:OD2	1:E:59:SER:HB3	2.20	0.42
1:F:208:GLY:O	1:F:211:ALA:HB3	2.19	0.42
1:A:169:ARG:O	1:A:197:GLN:HB2	2.20	0.42
1:B:2:PHE:CE2	1:B:75:PRO:HG3	2.55	0.42
1:C:107:ILE:HD11	1:D:104:PRO:HB3	2.01	0.42
1:C:37:ILE:HG23	1:C:226:THR:CG2	2.47	0.42
1:A:209:GLU:O	1:A:213:ARG:HG2	2.20	0.42
1:F:216:GLY:HA2	1:F:248:VAL:HG11	2.01	0.42
1:C:54:SER:OG	1:C:55:THR:N	2.52	0.42
1:C:27:GLU:CB	1:C:56:THR:HG21	2.47	0.42
1:D:206:ARG:O	1:D:241:ILE:HD11	2.19	0.42
1:B:249:LEU:CD2	1:B:249:LEU:H	2.27	0.42
1:E:63:ASN:O	1:E:66:ARG:HB3	2.20	0.42
1:F:237:LYS:HA	1:F:240:GLU:OE2	2.19	0.42
1:C:51:LEU:HA	1:C:51:LEU:HD12	1.89	0.41
1:A:161:MET:SD	1:E:119:LYS:HD3	2.60	0.41
1:E:18:LYS:HD2	1:E:215:ALA:HB1	2.01	0.41
1:F:238:ILE:O	1:F:241:ILE:HG22	2.21	0.41
1:F:66:ARG:HG3	1:F:89:TYR:CZ	2.55	0.41
1:C:169:ARG:HA	2:C:400:HOH:O	2.20	0.41
1:C:30:THR:HG22	1:C:33:GLU:OE1	2.19	0.41
1:B:162:GLU:OE2	1:F:111:GLN:HB2	2.19	0.41
1:E:247:SER:OG	1:E:247:SER:O	2.30	0.41
1:F:15:ARG:HB2	1:F:15:ARG:HE	1.58	0.41
1:B:248:VAL:HG12	1:B:249:LEU:N	2.35	0.41
1:F:96:MET:HA	1:F:128:MET:O	2.21	0.41
1:B:80:PRO:HD2	1:B:96:MET:CE	2.51	0.41
1:F:240:GLU:N	1:F:240:GLU:OE1	2.37	0.41
1:F:66:ARG:CG	1:F:89:TYR:CZ	3.04	0.41
1:E:13:ILE:HG21	1:E:19:ILE:HG12	2.02	0.41
1:C:66:ARG:NE	2:C:304:HOH:O	2.46	0.40
1:A:141:TRP:CH2	1:B:146:LYS:HE3	2.56	0.40
1:C:54:SER:HB3	2:C:301:HOH:O	2.21	0.40
1:D:241:ILE:O	1:D:245:MET:HE2	2.21	0.40
1:E:235:GLU:N	1:E:235:GLU:CD	2.75	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:101:SER:HA	1:F:145:THR:HA	2.04	0.40
1:D:209:GLU:O	1:D:213:ARG:HG3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	239/256 (93%)	234 (98%)	4 (2%)	1 (0%)	34 24
1	B	240/256 (94%)	238 (99%)	2 (1%)	0	100 100
1	C	238/256 (93%)	235 (99%)	3 (1%)	0	100 100
1	D	232/256 (91%)	218 (94%)	11 (5%)	3 (1%)	12 4
1	E	234/256 (91%)	223 (95%)	9 (4%)	2 (1%)	17 7
1	F	237/256 (93%)	228 (96%)	6 (2%)	3 (1%)	12 4
All	All	1420/1536 (92%)	1376 (97%)	35 (2%)	9 (1%)	25 13

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	236	ASP
1	F	247	SER
1	E	247	SER
1	D	55	THR
1	E	236	ASP
1	D	4	MET
1	F	236	ASP
1	F	108	ILE
1	D	108	ILE

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	190/203 (94%)	189 (100%)	1 (0%)	88	88
1	B	189/203 (93%)	185 (98%)	4 (2%)	53	41
1	C	188/203 (93%)	187 (100%)	1 (0%)	88	88
1	D	177/203 (87%)	173 (98%)	4 (2%)	50	38
1	E	181/203 (89%)	177 (98%)	4 (2%)	52	39
1	F	186/203 (92%)	184 (99%)	2 (1%)	73	67
All	All	1111/1218 (91%)	1095 (99%)	16 (1%)	67	58

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	172	TYR
1	B	56	THR
1	B	57	ASP
1	B	172	TYR
1	B	249	LEU
1	C	226	THR
1	D	55	THR
1	D	98	LEU
1	D	172	TYR
1	D	247	SER
1	E	66	ARG
1	E	172	TYR
1	E	235	GLU
1	E	247	SER
1	F	172	TYR
1	F	243	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	197	GLN

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Mol	Chain	Res	Type
1	D	63	ASN

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	243/256 (94%)	0.46	25 (10%) 6 10	25, 36, 55, 71	0
1	B	244/256 (95%)	0.70	31 (12%) 3 5	24, 38, 65, 80	0
1	C	242/256 (94%)	0.68	27 (11%) 5 8	24, 39, 61, 80	0
1	D	236/256 (92%)	1.43	68 (28%) 0 0	24, 55, 80, 90	0
1	E	238/256 (92%)	1.27	59 (24%) 0 0	24, 57, 79, 87	0
1	F	241/256 (94%)	1.22	54 (22%) 0 0	24, 53, 78, 84	0
All	All	1444/1536 (94%)	0.95	264 (18%) 1 1	24, 45, 75, 90	0

All (264) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	53	GLY	10.9
1	D	238	ILE	8.8
1	F	53	GLY	8.5
1	F	248	VAL	8.4
1	B	53	GLY	7.9
1	D	241	ILE	7.0
1	F	241	ILE	6.9
1	E	55	THR	6.7
1	E	248	VAL	6.6
1	C	227	VAL	6.6
1	C	228	VAL	6.6
1	F	226	THR	6.5
1	F	227	VAL	6.4
1	C	226	THR	6.4
1	B	249	LEU	6.2
1	F	55	THR	6.1
1	A	248	VAL	6.0
1	E	41	ALA	5.8
1	C	53	GLY	5.7

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Mol	Chain	Res	Type	RSRZ
1	D	214	VAL	5.5
1	F	1	MET	5.5
1	A	249	LEU	5.4
1	E	2	PHE	5.4
1	D	2	PHE	5.3
1	D	247	SER	5.2
1	E	53	GLY	5.2
1	D	1	MET	5.0
1	F	213	ARG	5.0
1	E	89	TYR	4.8
1	A	108	ILE	4.8
1	F	106	TRP	4.7
1	D	107	ILE	4.7
1	F	105	TYR	4.7
1	B	2	PHE	4.6
1	F	247	SER	4.6
1	D	84	THR	4.6
1	D	208	GLY	4.6
1	B	228	VAL	4.5
1	F	246	GLY	4.5
1	F	107	ILE	4.5
1	E	107	ILE	4.5
1	C	107	ILE	4.4
1	E	71	ASN	4.3
1	C	102	THR	4.3
1	A	102	THR	4.2
1	F	102	THR	4.2
1	B	102	THR	4.2
1	E	102	THR	4.1
1	B	107	ILE	4.1
1	D	16	GLU	4.1
1	B	227	VAL	4.0
1	F	99	LEU	4.0
1	C	142	VAL	4.0
1	D	105	TYR	4.0
1	B	55	THR	4.0
1	D	106	TRP	3.9
1	A	106	TRP	3.9
1	A	226	THR	3.8
1	F	108	ILE	3.8
1	A	105	TYR	3.8
1	D	101	SER	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	41	ALA	3.8
1	D	102	THR	3.8
1	A	228	VAL	3.8
1	E	247	SER	3.8
1	A	104	PRO	3.8
1	D	207	SER	3.7
1	C	55	THR	3.7
1	D	104	PRO	3.7
1	C	105	TYR	3.7
1	F	242	VAL	3.7
1	C	106	TRP	3.7
1	E	37	ILE	3.6
1	F	212	ALA	3.6
1	D	246	GLY	3.6
1	A	107	ILE	3.6
1	A	227	VAL	3.6
1	B	142	VAL	3.6
1	E	211	ALA	3.6
1	D	243	GLU	3.6
1	E	243	GLU	3.6
1	F	41	ALA	3.5
1	E	46	THR	3.5
1	D	37	ILE	3.5
1	E	145	THR	3.5
1	E	34	ALA	3.5
1	A	113	LEU	3.4
1	B	108	ILE	3.4
1	D	212	ALA	3.4
1	C	104	PRO	3.4
1	C	98	LEU	3.4
1	E	236	ASP	3.4
1	D	34	ALA	3.4
1	E	40	ALA	3.4
1	B	99	LEU	3.4
1	E	74	VAL	3.4
1	F	236	ASP	3.4
1	E	142	VAL	3.4
1	D	213	ARG	3.3
1	E	241	ILE	3.3
1	A	99	LEU	3.3
1	E	104	PRO	3.3
1	B	104	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	104	PRO	3.3
1	D	42	ILE	3.3
1	D	54	SER	3.3
1	E	108	ILE	3.2
1	C	234	VAL	3.2
1	E	207	SER	3.2
1	C	108	ILE	3.2
1	C	143	GLY	3.1
1	E	105	TYR	3.1
1	F	239	ARG	3.1
1	F	2	PHE	3.1
1	E	67	ALA	3.1
1	F	43	ARG	3.0
1	D	24	ILE	3.0
1	D	49	ILE	3.0
1	D	110	ALA	3.0
1	D	142	VAL	3.0
1	B	106	TRP	3.0
1	D	245	MET	3.0
1	F	141	TRP	3.0
1	F	44	GLY	3.0
1	D	69	ARG	3.0
1	E	43	ARG	3.0
1	C	101	SER	3.0
1	E	99	LEU	3.0
1	D	145	THR	2.9
1	F	238	ILE	2.9
1	B	105	TYR	2.9
1	D	67	ALA	2.9
1	A	101	SER	2.9
1	C	103	ASN	2.9
1	D	143	GLY	2.9
1	A	103	ASN	2.9
1	D	61	LEU	2.9
1	A	1	MET	2.9
1	E	212	ALA	2.9
1	A	142	VAL	2.9
1	D	206	ARG	2.9
1	F	110	ALA	2.9
1	C	1	MET	2.8
1	B	145	THR	2.8
1	E	103	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	101	SER	2.8
1	C	235	GLU	2.8
1	E	9	TYR	2.8
1	B	3	LYS	2.8
1	A	112	ALA	2.8
1	B	226	THR	2.8
1	E	106	TRP	2.8
1	E	45	GLY	2.8
1	E	143	GLY	2.7
1	F	143	GLY	2.7
1	D	98	LEU	2.7
1	D	144	ASP	2.7
1	F	103	ASN	2.7
1	B	141	TRP	2.7
1	B	101	SER	2.7
1	F	98	LEU	2.7
1	F	209	GLU	2.7
1	F	37	ILE	2.6
1	F	208	GLY	2.6
1	C	145	THR	2.6
1	D	30	THR	2.6
1	D	103	ASN	2.6
1	B	143	GLY	2.6
1	F	109	GLY	2.6
1	F	205	ILE	2.6
1	E	73	ASP	2.6
1	B	131	LEU	2.6
1	D	46	THR	2.6
1	A	145	THR	2.5
1	F	211	ALA	2.5
1	E	240	GLU	2.5
1	A	144	ASP	2.5
1	F	144	ASP	2.5
1	A	141	TRP	2.5
1	B	97	SER	2.5
1	E	238	ILE	2.5
1	F	39	ARG	2.5
1	B	73	ASP	2.5
1	D	72	ILE	2.5
1	E	182	HIS	2.5
1	D	32	GLU	2.5
1	E	66	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	248	VAL	2.4
1	D	58	SER	2.4
1	F	145	THR	2.4
1	D	237	LYS	2.4
1	F	243	GLU	2.4
1	A	143	GLY	2.4
1	B	98	LEU	2.4
1	C	144	ASP	2.4
1	D	70	GLU	2.4
1	F	235	GLU	2.4
1	C	110	ALA	2.3
1	D	40	ALA	2.3
1	E	70	GLU	2.3
1	F	240	GLU	2.3
1	E	24	ILE	2.3
1	E	36	GLU	2.3
1	D	65	ALA	2.3
1	D	211	ALA	2.3
1	D	31	PRO	2.3
1	B	144	ASP	2.3
1	D	209	GLU	2.3
1	F	101	SER	2.3
1	A	110	ALA	2.3
1	E	112	ALA	2.3
1	A	109	GLY	2.3
1	D	240	GLU	2.3
1	F	30	THR	2.3
1	D	97	SER	2.3
1	D	71	ASN	2.2
1	B	110	ALA	2.2
1	D	25	ASP	2.2
1	F	142	VAL	2.2
1	C	113	LEU	2.2
1	C	131	LEU	2.2
1	E	88	ARG	2.2
1	D	38	ALA	2.2
1	C	97	SER	2.2
1	C	247	SER	2.2
1	B	81	GLY	2.2
1	E	246	GLY	2.2
1	D	131	LEU	2.2
1	E	110	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	206	ARG	2.2
1	E	10	PHE	2.2
1	E	242	VAL	2.2
1	D	112	ALA	2.1
1	D	181	GLU	2.1
1	C	193	ARG	2.1
1	E	13	ILE	2.1
1	E	215	ALA	2.1
1	E	54	SER	2.1
1	D	118	VAL	2.1
1	F	245	MET	2.1
1	D	99	LEU	2.1
1	A	97	SER	2.1
1	E	146	LYS	2.1
1	D	89	TYR	2.1
1	D	56	THR	2.1
1	F	54	SER	2.1
1	B	100	ASN	2.1
1	E	100	ASN	2.1
1	D	36	GLU	2.1
1	D	109	GLY	2.1
1	D	55	THR	2.1
1	E	245	MET	2.1
1	E	141	TRP	2.1
1	E	131	LEU	2.1
1	F	113	LEU	2.1
1	F	40	ALA	2.0
1	B	147	PRO	2.0
1	B	103	ASN	2.0
1	F	59	SER	2.0
1	E	209	GLU	2.0
1	F	112	ALA	2.0
1	D	108	ILE	2.0
1	E	113	LEU	2.0
1	F	42	ILE	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.