



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:56 AM UTC

PDB ID : 5NDY / pdb_00005ndy
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 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

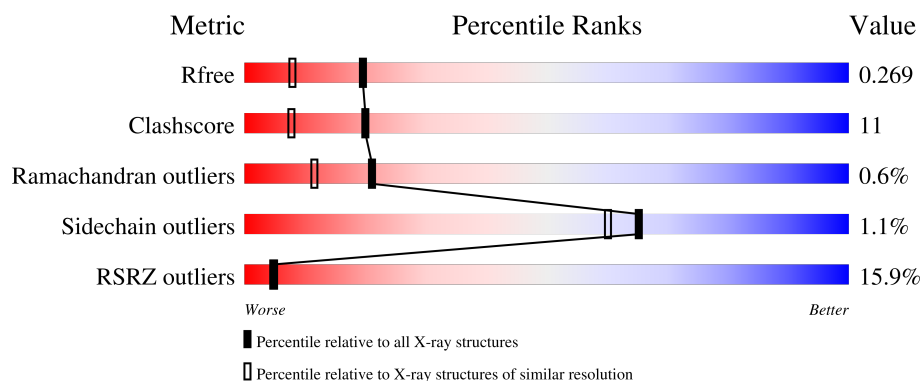
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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	256	5% 84% 10% • 5%
1	B	256	9% 81% 13% • 5%
1	C	256	6% 83% 11% 5%
1	D	256	29% 68% 22% • 8%
1	E	256	24% 70% 21% • 7%

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Mol	Chain	Length	Quality of chain
1	F	256	16% 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

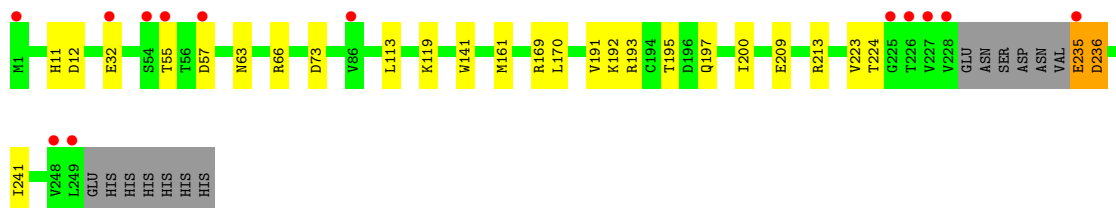
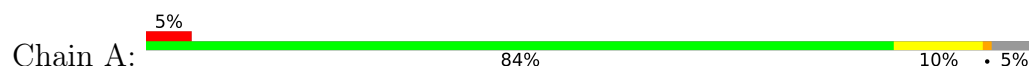
- Molecule 2 is water.

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

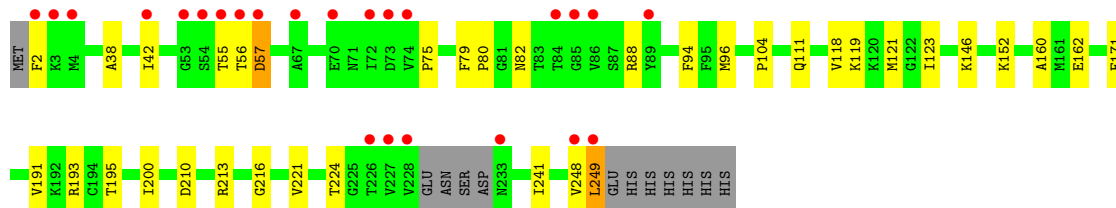
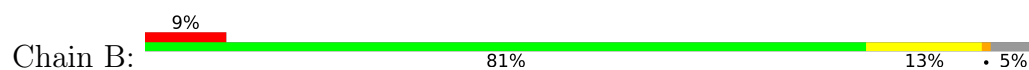
3 Residue-property plots [i](#)

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.

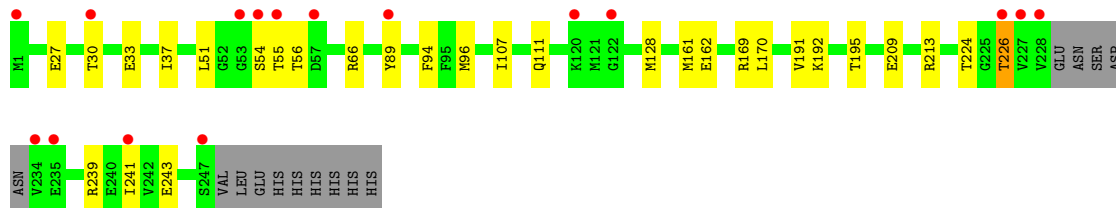
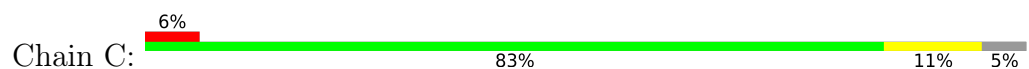
- Molecule 1: Geranylgeranylglyceryl phosphate synthase



- Molecule 1: Geranylgeranylglyceryl phosphate synthase

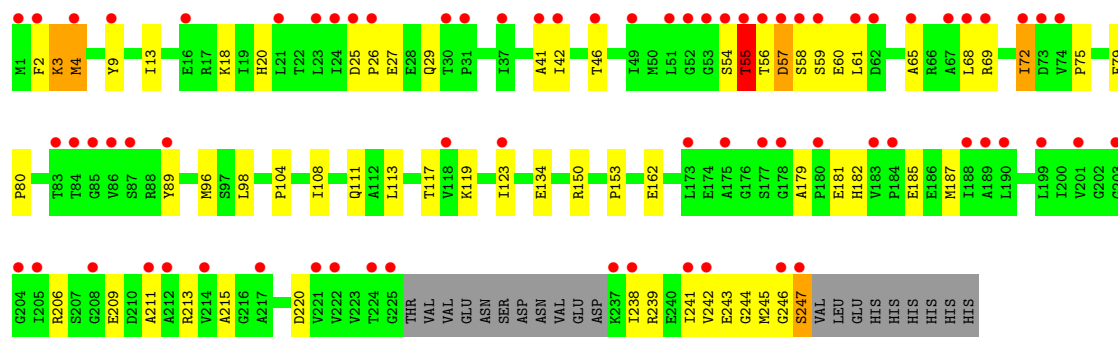


- Molecule 1: Geranylgeranylglyceryl phosphate synthase

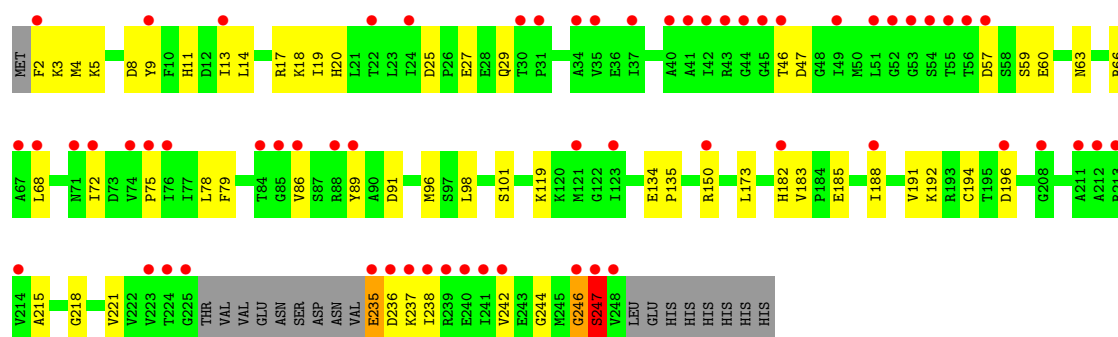


- Molecule 1: Geranylgeranylglyceryl phosphate synthase

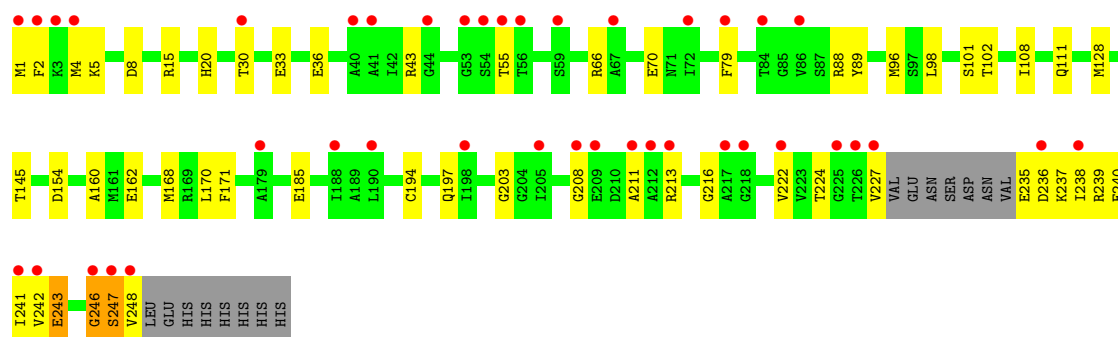
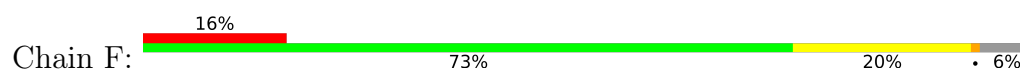




- Molecule 1: Geranylgeranylglyceryl phosphate synthase



- Molecule 1: Geranylgeranylglyceryl phosphate synthase



4 Data and refinement statistics

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) 97.4 (49.77-1.95)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.01 (at 1.95Å)	Xtriage
Refinement program	PHENIX (1.10pre_2119: ???)	Depositor
R, R_{free}	0.218 , 0.262 0.237 , 0.269	Depositor DCC
R_{free} test set	6259 reflections (4.87%)	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)	0.36 , 39.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

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	0.52	1/1855 (0.1%)	0.64	1/2513 (0.0%)
1	B	0.51	0/1854	0.57	0/2514
1	C	0.48	0/1843	0.56	0/2498
1	D	0.41	0/1780	0.69	3/2415 (0.1%)
1	E	0.36	0/1798	0.54	2/2440 (0.1%)
1	F	0.44	0/1832	0.62	1/2484 (0.0%)
All	All	0.45	1/10962 (0.0%)	0.60	7/14864 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	223	VAL	C-O	-5.19	1.18	1.24

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	56	THR	N-CA-C	12.17	125.53	108.74
1	D	57	ASP	N-CA-C	-7.77	97.97	110.32
1	D	3	LYS	N-CA-C	-6.27	97.45	110.80
1	E	246	GLY	N-CA-C	-5.96	99.05	113.18
1	F	246	GLY	N-CA-C	-5.86	105.19	111.93
1	A	235	GLU	N-CA-C	-5.32	96.11	111.00
1	E	3	LYS	N-CA-C	5.05	118.59	112.23

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	1825	0	1834	22	0
1	B	1824	0	1821	31	0
1	C	1813	0	1812	29	0
1	D	1750	0	1727	64	0
1	E	1768	0	1742	53	0
1	F	1802	0	1792	61	0
2	A	145	0	0	7	0
2	B	132	0	0	1	0
2	C	122	0	0	5	0
2	D	45	0	0	3	0
2	E	60	0	0	9	0
2	F	45	0	0	3	0
All	All	11331	0	10728	245	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 (245) 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:4:MET:HE3	1:F:5:LYS:HB2	1.39	1.05
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:LYS:NZ	1:F:194:CYS:O	2.14	0.80
1:B:80:PRO:HD2	1:B:96:MET:HE3	1.64	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
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:18:LYS:NZ	2:E:305:HOH:O	2.17	0.77
1:D:241:ILE:HG22	1:D:245:MET:HE2	1.65	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: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:F:4:MET:HE3	1:F:5:LYS:CB	2.18	0.72
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:HG3	1:D:206:ARG:HH11	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:134:GLU:OE2	2:D:302:HOH:O	2.12	0.68
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:D:80:PRO:HD2	1:D:96:MET:HE3	1.77	0.67
1:A:73:ASP:OD2	2:A:302:HOH:O	2.12	0.66
1:F:4:MET:HE3	1:F:5:LYS:H	1.61	0.65
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:54:SER:HB2	1:D:55:THR:C	2.22	0.64
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:235:GLU:O	1:E:237:LYS:N	2.29	0.62
1:B:79:PHE:CD1	1:B:96:MET:HE1	2.34	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:D:242:VAL:HA	1:D:245:MET:HE3	1.82	0.61
1:B:210:ASP:OD1	1:B:213:ARG:NH2	2.34	0.60
1:E:244:GLY:C	1:E:246:GLY:H	2.09	0.60
1:B:249:LEU:HD22	1:B:249:LEU:H	1.67	0.60
1:D:2:PHE:CZ	1:D:75:PRO:HG3	2.36	0.60
1:D:54:SER:CB	1:D:55:THR:HB	2.32	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:246:GLY:HA2	1:D:247:SER:C	2.26	0.59
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:F:4:MET:HE2	1:F:8:ASP:HB2	1.85	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:F:235:GLU:C	1:F:237:LYS:H	2.12	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:E:235:GLU:C	1:E:237:LYS:H	2.13	0.57
1:A:57:ASP:OD2	2:F:303:HOH:O	2.17	0.57
1:D:79:PHE:CD1	1:D:96:MET:HE1	2.39	0.57
1:D:26:PRO:HG3	1:D:61:LEU:CD1	2.29	0.57
1:E:235:GLU:N	1:E:235:GLU:OE2	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:20:HIS:HB2	1:D:245:MET:HE1	1.90	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:C:94:PHE:HB3	1:C:96:MET:HE3	1.89	0.53
1:F:160:ALA:HA	1:F:171:PHE:CE1	2.44	0.52
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:A:235:GLU:CG	1:A:236:ASP:H	2.20	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: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: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	1.96	0.48
1:F:4:MET:CE	1:F:5:LYS:HB2	2.28	0.48
1:E:247:SER:O	1:E:247:SER:OG	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:68:LEU:HD23	1:D:68:LEU:HA	1.63	0.47
1:D:206:ARG:HH11	1:D:206:ARG:CG	2.25	0.47
1:E:244:GLY:C	1:E:246:GLY:N	2.72	0.46
1:C:94:PHE:CE1	1:C:128:MET:HE1	2.51	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:A:55:THR:O	1:A:55:THR:OG1	2.29	0.45
1:F:30:THR:N	1:F:33:GLU:OE2	2.36	0.45
1:F:79:PHE:CE1	1:F:96:MET:HE1	2.51	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:E:235:GLU:N	1:E:235:GLU:CD	2.75	0.45
1:A:32:GLU:HG3	2:A:343:HOH:O	2.17	0.45
1:D:20:HIS:ND1	1:D:46:THR:OG1	2.39	0.44
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:D:54:SER:C	1:D:55:THR:OG1	2.58	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:D:18:LYS:HD3	1:D:215:ALA:HB1	2.00	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:79:PHE:CE1	1:E:96:MET:HE1	2.52	0.44
1:E:27:GLU:HA	1:E:60:GLU:OE2	2.18	0.44
1:E:238:ILE:CG2	1:E:242:VAL:HG23	2.44	0.44
1:F:98:LEU:HG	1:F:101:SER:HB2	1.99	0.44
1:A:113:LEU:HD22	1:F:55:THR:HB	2.00	0.43
1:D:27:GLU:HG3	1:D:60:GLU:OE1	2.18	0.43
1:D:206:ARG:HG3	1:D:206:ARG:NH1	2.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:MET:HE2	1:C:170:LEU:CB	2.47	0.43
1:F:240:GLU:HA	1:F:243:GLU:CB	2.48	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:CG	1:D:206:ARG:NH1	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:B:94:PHE:HB3	1:B:96:MET:HE2	2.01	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
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:57:ASP:OD2	1:E:59:SER:HB3	2.20	0.42
1:E:134:GLU:CG	1:E:150:ARG:HG3	2.45	0.42
1:F:128:MET:HE2	1:F:170:LEU:HB3	2.02	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:37:ILE:HG23	1:C:226:THR:CG2	2.47	0.42
1:C:107:ILE:HD11	1:D:104:PRO:HB3	2.01	0.42
1:A:209:GLU:O	1:A:213:ARG:HG2	2.20	0.42
1:F:128:MET:HE3	1:F:128:MET:HB2	1.72	0.42
1:F:216:GLY:HA2	1:F:248:VAL:HG11	2.01	0.42
1:C:27:GLU:CB	1:C:56:THR:HG21	2.47	0.42
1:C:54:SER:OG	1:C:55:THR:N	2.52	0.42
1:D:206:ARG:O	1:D:241:ILE:HD11	2.19	0.42
1:B:249:LEU:H	1:B:249:LEU:CD2	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:F:79:PHE:CD1	1:F:96:MET:HE1	2.55	0.42
1:A:161:MET:SD	1:E:119:LYS:HD3	2.60	0.41
1:C:51:LEU:HD12	1:C:51:LEU:HA	1.89	0.41
1:E:18:LYS:HD2	1:E:215:ALA:HB1	2.01	0.41
1:F:4:MET:HE3	1:F:5:LYS:N	2.30	0.41
1:F:66:ARG:HG3	1:F:89:TYR:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:238:ILE:O	1:F:241:ILE:HG22	2.21	0.41
1:C:30:THR:HG22	1:C:33:GLU:OE1	2.19	0.41
1:C:128:MET:HE3	1:C:128:MET:HB2	1.91	0.41
1:C:169:ARG:HA	2:C:400:HOH:O	2.20	0.41
1:F:4:MET:HE2	1:F:8:ASP:CB	2.50	0.41
1:B:162:GLU:OE2	1:F:111:GLN:HB2	2.19	0.41
1:F:15:ARG:HE	1:F:15:ARG:HB2	1.58	0.41
1:B:248:VAL:HG12	1:B:249:LEU:N	2.35	0.41
1:D:153:PRO:HA	1:D:187:MET:HE2	2.00	0.41
1:F:96:MET:HA	1:F:128:MET:O	2.21	0.41
1:E:4:MET:HE3	1:E:4:MET:HB2	1.80	0.41
1:E:235:GLU:C	1:E:237:LYS:N	2.72	0.41
1:F:66:ARG:CG	1:F:89:TYR:CZ	3.04	0.41
1:F:240:GLU:OE1	1:F:240:GLU:N	2.37	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:244:GLY:C	1:D:246:GLY:H	2.30	0.40
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%)	30	22
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%)	9	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	234/256 (91%)	223 (95%)	9 (4%)	2 (1%)	14	6
1	F	237/256 (93%)	228 (96%)	6 (2%)	3 (1%)	9	3
All	All	1420/1536 (92%)	1376 (97%)	35 (2%)	9 (1%)	21	11

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 ⓘ

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%)	190 (100%)	0	100	100
1	B	189/203 (93%)	186 (98%)	3 (2%)	55	46
1	C	188/203 (93%)	187 (100%)	1 (0%)	81	82
1	D	177/203 (87%)	173 (98%)	4 (2%)	44	33
1	E	181/203 (89%)	179 (99%)	2 (1%)	65	60
1	F	186/203 (92%)	184 (99%)	2 (1%)	65	60
All	All	1111/1218 (91%)	1099 (99%)	12 (1%)	65	60

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	56	THR

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Mol	Chain	Res	Type
1	B	57	ASP
1	B	249	LEU
1	C	226	THR
1	D	55	THR
1	D	72	ILE
1	D	98	LEU
1	D	247	SER
1	E	235	GLU
1	E	247	SER
1	F	227	VAL
1	F	243	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	ASN
1	A	197	GLN
1	B	197	GLN
1	C	197	GLN
1	D	63	ASN
1	E	63	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	243/256 (94%)	0.46	13 (5%) 32 36	25, 36, 55, 71	0
1	B	244/256 (95%)	0.68	24 (9%) 13 14	24, 38, 65, 80	0
1	C	242/256 (94%)	0.62	16 (6%) 24 27	24, 39, 61, 80	0
1	D	236/256 (92%)	1.55	73 (30%) 1 1	24, 55, 80, 90	0
1	E	238/256 (92%)	1.44	62 (26%) 1 1	24, 57, 79, 87	0
1	F	241/256 (94%)	1.28	41 (17%) 4 4	24, 53, 78, 84	0
All	All	1444/1536 (94%)	1.00	229 (15%) 5 5	24, 45, 75, 90	0

All (229) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	53	GLY	7.2
1	D	53	GLY	7.0
1	F	53	GLY	6.6
1	C	226	THR	6.3
1	F	1	MET	5.9
1	F	248	VAL	5.9
1	F	226	THR	5.7
1	F	55	THR	5.6
1	C	228	VAL	5.5
1	C	227	VAL	5.5
1	B	55	THR	5.4
1	E	55	THR	5.4
1	B	53	GLY	5.3
1	D	2	PHE	5.3
1	F	241	ILE	5.2
1	E	248	VAL	5.2
1	E	2	PHE	5.1
1	B	2	PHE	5.0
1	E	53	GLY	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	248	VAL	4.9
1	F	227	VAL	4.9
1	D	84	THR	4.7
1	E	41	ALA	4.7
1	D	247	SER	4.6
1	C	55	THR	4.5
1	B	249	LEU	4.4
1	D	238	ILE	4.4
1	E	236	ASP	4.2
1	A	226	THR	4.2
1	B	228	VAL	4.2
1	D	42	ILE	4.2
1	E	246	GLY	4.2
1	E	225	GLY	4.1
1	F	247	SER	4.0
1	D	4	MET	4.0
1	D	246	GLY	3.9
1	D	74	VAL	3.9
1	B	227	VAL	3.8
1	E	24	ILE	3.7
1	E	241	ILE	3.7
1	D	214	VAL	3.7
1	E	89	TYR	3.6
1	F	2	PHE	3.6
1	D	61	LEU	3.6
1	A	55	THR	3.6
1	D	54	SER	3.6
1	D	56	THR	3.5
1	A	249	LEU	3.5
1	D	51	LEU	3.5
1	A	54	SER	3.5
1	D	241	ILE	3.5
1	A	1	MET	3.4
1	D	55	THR	3.4
1	E	46	THR	3.4
1	D	237	LYS	3.4
1	B	226	THR	3.4
1	B	73	ASP	3.4
1	E	247	SER	3.4
1	C	1	MET	3.4
1	D	72	ILE	3.3
1	D	242	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	190	LEU	3.3
1	D	208	GLY	3.3
1	C	235	GLU	3.3
1	D	41	ALA	3.2
1	E	67	ALA	3.2
1	C	54	SER	3.2
1	D	65	ALA	3.2
1	F	212	ALA	3.2
1	E	45	GLY	3.2
1	A	228	VAL	3.2
1	E	86	VAL	3.2
1	E	56	THR	3.1
1	B	3	LYS	3.1
1	E	54	SER	3.1
1	E	44	GLY	3.1
1	E	74	VAL	3.1
1	E	123	ILE	3.1
1	D	1	MET	3.0
1	E	31	PRO	3.0
1	D	205	ILE	3.0
1	E	22	THR	2.9
1	E	40	ALA	2.9
1	E	212	ALA	2.9
1	D	68	LEU	2.9
1	F	59	SER	2.9
1	F	86	VAL	2.9
1	D	16	GLU	2.9
1	D	24	ILE	2.9
1	A	227	VAL	2.8
1	B	56	THR	2.8
1	F	242	VAL	2.8
1	D	217	ALA	2.8
1	D	211	ALA	2.8
1	B	85	GLY	2.8
1	F	84	THR	2.8
1	E	242	VAL	2.8
1	D	30	THR	2.7
1	C	57	ASP	2.7
1	E	13	ILE	2.7
1	D	184	PRO	2.7
1	D	222	VAL	2.7
1	F	40	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	4	MET	2.7
1	F	238	ILE	2.7
1	E	71	ASN	2.7
1	F	236	ASP	2.7
1	E	76	ILE	2.7
1	D	85	GLY	2.6
1	E	43	ARG	2.6
1	E	188	ILE	2.6
1	D	225	GLY	2.6
1	F	222	VAL	2.6
1	E	239	ARG	2.6
1	F	179	ALA	2.6
1	F	3	LYS	2.6
1	F	72	ILE	2.6
1	F	213	ARG	2.6
1	B	84	THR	2.6
1	E	213	ARG	2.6
1	A	57	ASP	2.6
1	F	205	ILE	2.6
1	D	86	VAL	2.6
1	E	211	ALA	2.6
1	B	54	SER	2.6
1	F	54	SER	2.5
1	F	56	THR	2.5
1	D	26	PRO	2.5
1	E	9	TYR	2.5
1	D	59	SER	2.5
1	D	189	ALA	2.5
1	A	235	GLU	2.5
1	D	57	ASP	2.5
1	F	225	GLY	2.5
1	C	247	SER	2.5
1	D	188	ILE	2.5
1	F	30	THR	2.5
1	D	201	VAL	2.5
1	E	237	LYS	2.5
1	E	85	GLY	2.4
1	C	30	THR	2.4
1	D	62	ASP	2.4
1	D	73	ASP	2.4
1	E	35	VAL	2.4
1	E	214	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	21	LEU	2.4
1	D	23	LEU	2.4
1	B	42	ILE	2.4
1	D	49	ILE	2.4
1	F	218	GLY	2.4
1	E	84	THR	2.4
1	E	49	ILE	2.4
1	F	211	ALA	2.4
1	C	122	GLY	2.4
1	F	246	GLY	2.4
1	E	51	LEU	2.3
1	F	79	PHE	2.3
1	D	46	THR	2.3
1	D	37	ILE	2.3
1	E	37	ILE	2.3
1	E	42	ILE	2.3
1	D	177	SER	2.3
1	D	9	TYR	2.3
1	B	233	ASN	2.3
1	B	248	VAL	2.3
1	D	221	VAL	2.3
1	D	83	THR	2.3
1	D	212	ALA	2.3
1	D	52	GLY	2.3
1	D	123	ILE	2.3
1	E	52	GLY	2.3
1	E	72	ILE	2.3
1	E	57	ASP	2.3
1	E	196	ASP	2.3
1	A	86	VAL	2.3
1	D	173	LEU	2.3
1	B	89	TYR	2.2
1	D	175	ALA	2.2
1	C	241	ILE	2.2
1	D	118	VAL	2.2
1	B	70	GLU	2.2
1	D	199	LEU	2.2
1	D	69	ARG	2.2
1	D	58	SER	2.2
1	D	203	GLY	2.2
1	B	72	ILE	2.2
1	E	88	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	32	GLU	2.2
1	B	74	VAL	2.2
1	C	234	VAL	2.2
1	E	223	VAL	2.2
1	A	225	GLY	2.2
1	D	178	GLY	2.2
1	D	204	GLY	2.2
1	E	68	LEU	2.2
1	E	208	GLY	2.2
1	E	240	GLU	2.1
1	F	198	ILE	2.1
1	E	224	THR	2.1
1	D	31	PRO	2.1
1	F	41	ALA	2.1
1	E	238	ILE	2.1
1	D	87	SER	2.1
1	B	86	VAL	2.1
1	D	183	VAL	2.1
1	C	120	LYS	2.1
1	D	67	ALA	2.1
1	C	89	TYR	2.1
1	E	150	ARG	2.1
1	E	30	THR	2.1
1	E	235	GLU	2.1
1	F	209	GLU	2.1
1	F	67	ALA	2.1
1	F	217	ALA	2.1
1	F	188	ILE	2.0
1	D	224	THR	2.0
1	E	182	HIS	2.0
1	F	190	LEU	2.0
1	B	67	ALA	2.0
1	E	34	ALA	2.0
1	B	57	ASP	2.0
1	D	25	ASP	2.0
1	B	4	MET	2.0
1	E	121	MET	2.0
1	F	44	GLY	2.0
1	F	208	GLY	2.0
1	D	89	TYR	2.0
1	D	180	PRO	2.0
1	E	75	PRO	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.