



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 05:14 AM UTC

PDB ID : 5HEG / pdb_00005heg
Title : Pentameric ligand-gated ion channel GLIC mutant P246G
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Deposited on : 2016-01-06
Resolution : 3.21 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

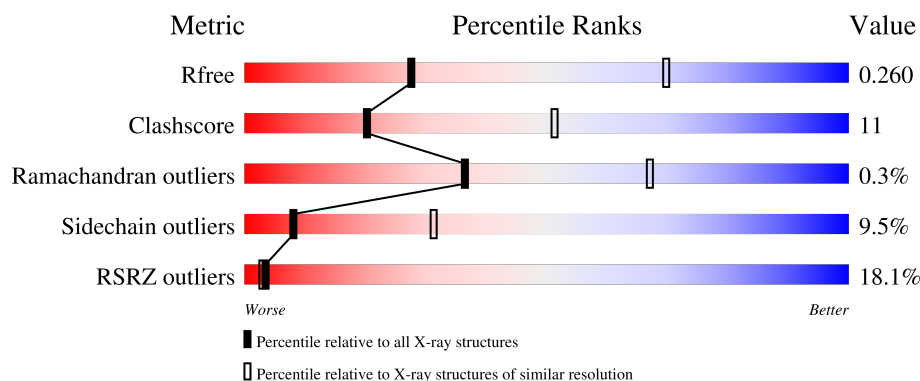
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.21 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	1768 (3.24-3.20)
Clashscore	190562	1879 (3.24-3.20)
Ramachandran outliers	187476	1844 (3.24-3.20)
Sidechain outliers	187428	1843 (3.24-3.20)
RSRZ outliers	180081	1768 (3.24-3.20)

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	316	20% 66% 28% ..
1	B	316	21% 66% 28% ..
1	C	316	15% 67% 28% ..
1	D	316	18% 64% 29% ..
1	E	316	15% 66% 28% ..

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12590 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 Proton-gated ion channel.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2518	1659	403	452	4			
1	B	310	Total	C	N	O	S	0	0	0
			2518	1659	403	452	4			
1	C	310	Total	C	N	O	S	0	0	0
			2518	1659	403	452	4			
1	D	310	Total	C	N	O	S	0	0	0
			2518	1659	403	452	4			
1	E	310	Total	C	N	O	S	0	0	0
			2518	1659	403	452	4			

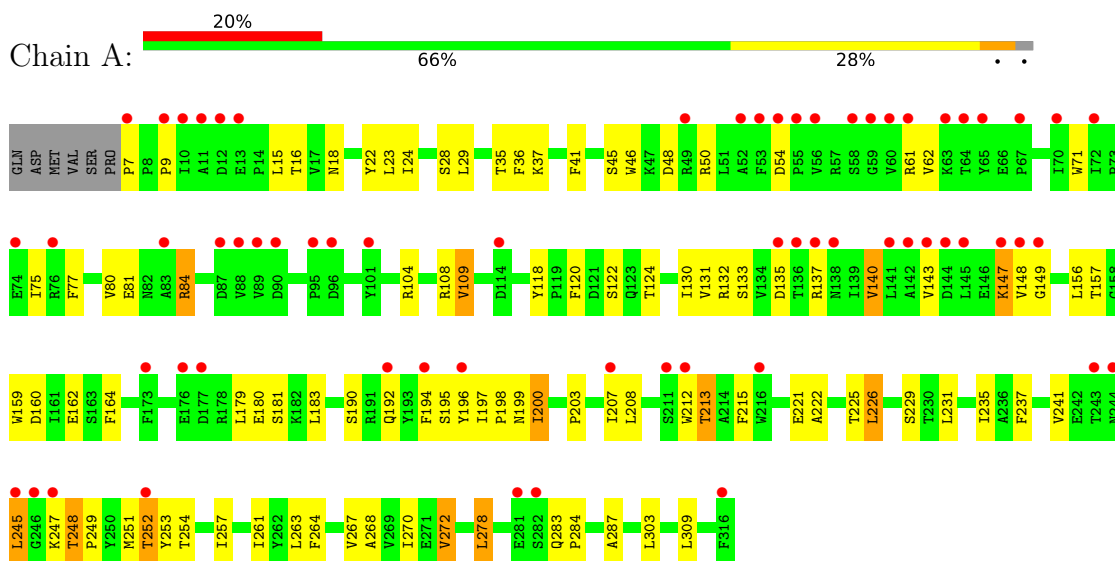
There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	246	GLY	PRO	engineered mutation	UNP Q7NDN8
B	246	GLY	PRO	engineered mutation	UNP Q7NDN8
C	246	GLY	PRO	engineered mutation	UNP Q7NDN8
D	246	GLY	PRO	engineered mutation	UNP Q7NDN8
E	246	GLY	PRO	engineered mutation	UNP Q7NDN8

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.

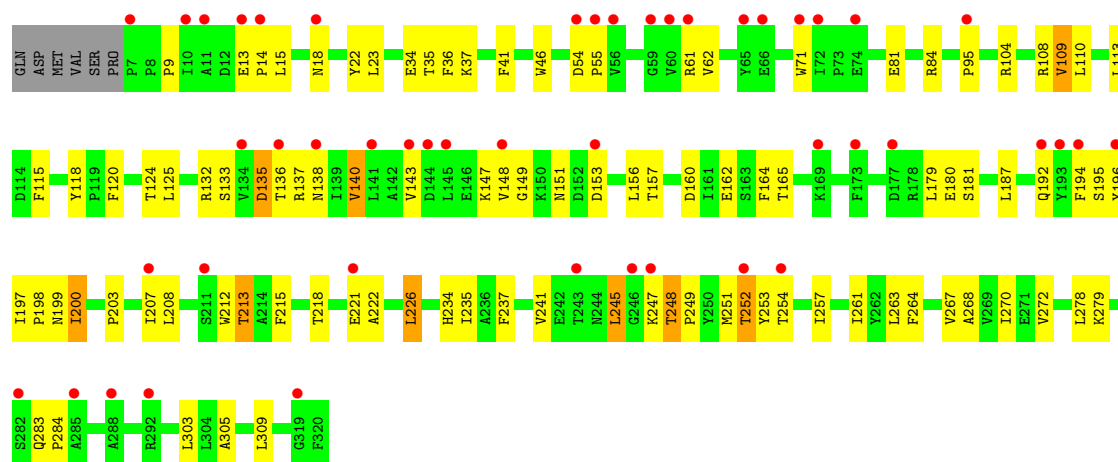
- Molecule 1: Proton-gated ion channel



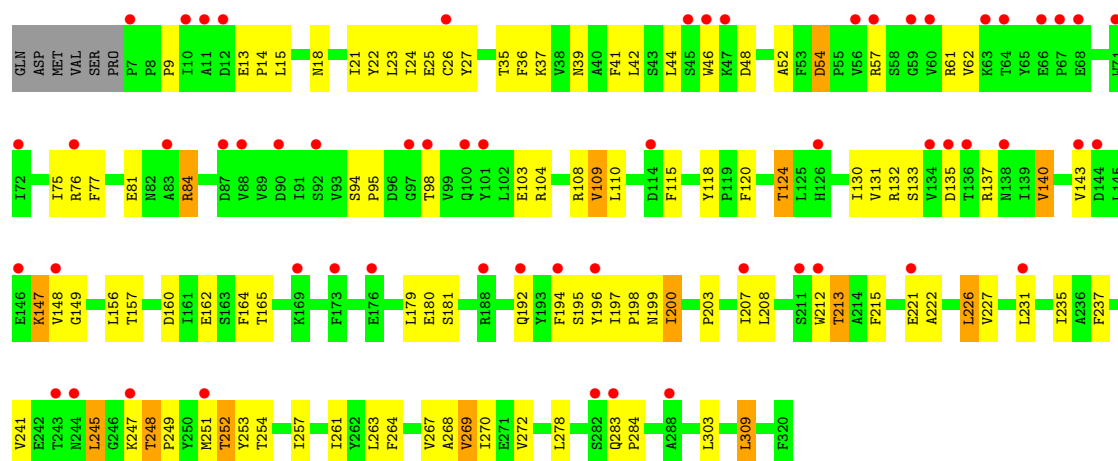
- Molecule 1: Proton-gated ion channel



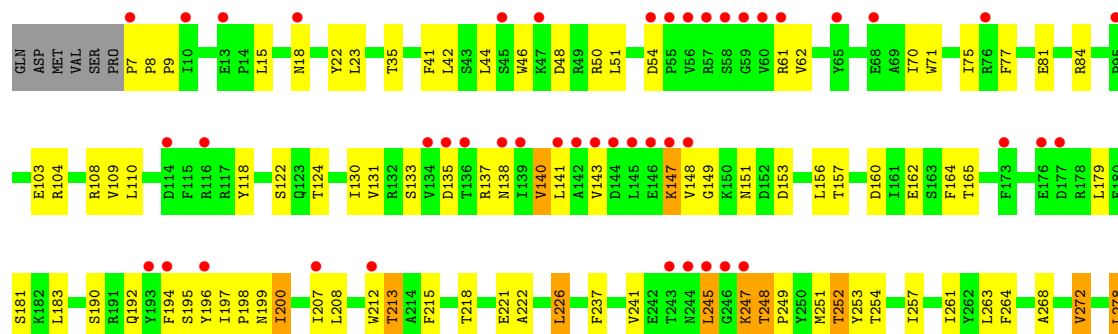
- Molecule 1: Proton-gated ion channel

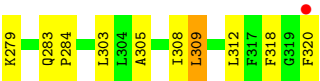


• Molecule 1: Proton-gated ion channel



• Molecule 1: Proton-gated ion channel





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	180.38Å 134.21Å 160.79Å 90.00° 101.97° 90.00°	Depositor
Resolution (Å)	29.92 – 3.21 29.92 – 3.21	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.92-3.21) 99.5 (29.92-3.21)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.10_2155	Depositor
R, R_{free}	0.247 , 0.258 0.252 , 0.260	Depositor DCC
R_{free} test set	2801 reflections (4.59%)	wwPDB-VP
Wilson B-factor (Å ²)	83.2	Xtriage
Anisotropy	0.372	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 55.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	12590	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.86% 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	0.17	0/2585	0.43	0/3528
1	B	0.19	0/2585	0.43	0/3528
1	C	0.18	0/2585	0.43	0/3528
1	D	0.18	0/2585	0.44	0/3528
1	E	0.18	0/2585	0.43	0/3528
All	All	0.18	0/12925	0.43	0/17640

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2518	0	2533	64	0
1	B	2518	0	2533	60	0
1	C	2518	0	2533	59	0
1	D	2518	0	2533	66	0
1	E	2518	0	2533	59	0
All	All	12590	0	12665	286	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 (286) 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:22:TYR:HA	1:B:149:GLY:HA2	1.55	0.88
1:D:22:TYR:HA	1:D:149:GLY:HA2	1.57	0.86
1:E:22:TYR:HA	1:E:149:GLY:HA2	1.56	0.86
1:C:22:TYR:HA	1:C:149:GLY:HA2	1.60	0.81
1:A:22:TYR:HA	1:A:149:GLY:HA2	1.63	0.79
1:B:147:LYS:O	1:B:149:GLY:N	2.19	0.76
1:D:147:LYS:O	1:D:149:GLY:N	2.19	0.74
1:E:196:TYR:HA	1:E:200:ILE:HG12	1.70	0.74
1:B:196:TYR:HA	1:B:200:ILE:HG12	1.69	0.74
1:E:147:LYS:O	1:E:149:GLY:N	2.21	0.74
1:D:15:LEU:HD11	1:D:46:TRP:HB2	1.73	0.70
1:D:196:TYR:HA	1:D:200:ILE:HG12	1.73	0.70
1:C:147:LYS:O	1:C:149:GLY:N	2.24	0.70
1:C:196:TYR:HA	1:C:200:ILE:HG12	1.75	0.69
1:A:147:LYS:O	1:A:149:GLY:N	2.26	0.69
1:A:18:ASN:HB3	1:A:143:VAL:HG23	1.77	0.66
1:A:200:ILE:HG23	1:A:241:VAL:HG11	1.79	0.65
1:E:257:ILE:HG22	1:E:309:LEU:HD23	1.78	0.65
1:D:18:ASN:HB3	1:D:143:VAL:HG23	1.78	0.64
1:A:196:TYR:HA	1:A:200:ILE:HG12	1.78	0.64
1:C:200:ILE:HG23	1:C:241:VAL:HG11	1.80	0.63
1:D:104:ARG:NH1	1:E:77:PHE:O	2.30	0.63
1:B:257:ILE:HG22	1:B:309:LEU:HD23	1.80	0.63
1:A:235:ILE:HD13	1:E:237:PHE:HB2	1.80	0.62
1:B:18:ASN:HB3	1:B:143:VAL:HG23	1.82	0.62
1:C:18:ASN:HB3	1:C:143:VAL:HG23	1.81	0.61
1:E:15:LEU:HD11	1:E:46:TRP:HB2	1.82	0.61
1:B:147:LYS:HE2	1:B:165:THR:HA	1.83	0.61
1:B:22:TYR:HB3	1:B:41:PHE:HB2	1.82	0.61
1:A:251:MET:HB2	1:E:194:PHE:CE1	2.36	0.61
1:B:213:THR:HG22	1:B:226:LEU:HD11	1.83	0.61
1:A:213:THR:HG22	1:A:226:LEU:HD11	1.82	0.61
1:E:147:LYS:HE2	1:E:165:THR:HA	1.83	0.60
1:B:15:LEU:HD11	1:B:46:TRP:HB2	1.83	0.60
1:B:151:ASN:ND2	1:B:153:ASP:OD1	2.32	0.60
1:A:104:ARG:NH1	1:B:77:PHE:O	2.32	0.59
1:E:200:ILE:HG23	1:E:241:VAL:HG11	1.82	0.59
1:D:194:PHE:CE1	1:E:251:MET:HB2	2.38	0.59
1:C:237:PHE:HB2	1:D:235:ILE:HD13	1.84	0.58
1:E:35:THR:OG1	1:E:108:ARG:NH2	2.37	0.58
1:A:22:TYR:HB3	1:A:41:PHE:HB2	1.84	0.58
1:B:257:ILE:O	1:B:261:ILE:HG12	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:LEU:HD11	1:A:46:TRP:HB2	1.86	0.58
1:D:22:TYR:HB3	1:D:41:PHE:HB2	1.84	0.58
1:A:257:ILE:HG22	1:A:309:LEU:HD23	1.86	0.58
1:D:54:ASP:HB2	1:D:57:ARG:HB2	1.85	0.58
1:D:257:ILE:O	1:D:261:ILE:HG12	2.04	0.58
1:A:35:THR:OG1	1:A:108:ARG:NH2	2.38	0.57
1:D:37:LYS:HG3	1:D:108:ARG:HB3	1.87	0.57
1:B:23:LEU:N	1:B:149:GLY:O	2.36	0.57
1:C:23:LEU:N	1:C:149:GLY:O	2.38	0.57
1:C:151:ASN:ND2	1:C:153:ASP:OD1	2.38	0.57
1:B:194:PHE:CE1	1:C:251:MET:HB2	2.38	0.57
1:A:257:ILE:O	1:A:261:ILE:HG12	2.05	0.57
1:B:157:THR:OG1	1:C:34:GLU:OE1	2.17	0.56
1:B:200:ILE:HG23	1:B:241:VAL:HG11	1.87	0.56
1:E:140:VAL:HG22	1:E:181:SER:HB3	1.87	0.56
1:C:81:GLU:HG3	1:C:108:ARG:HG3	1.87	0.56
1:D:200:ILE:HG23	1:D:241:VAL:HG11	1.87	0.56
1:D:81:GLU:HG3	1:D:108:ARG:HG3	1.87	0.56
1:E:18:ASN:HB3	1:E:143:VAL:HG23	1.87	0.56
1:D:23:LEU:N	1:D:149:GLY:O	2.38	0.56
1:E:151:ASN:ND2	1:E:153:ASP:OD1	2.38	0.56
1:A:194:PHE:CE1	1:B:251:MET:HB2	2.41	0.55
1:E:118:TYR:CD1	1:E:245:LEU:HD11	2.41	0.55
1:A:37:LYS:HG3	1:A:108:ARG:HB3	1.89	0.55
1:B:81:GLU:HG3	1:B:108:ARG:HG3	1.89	0.55
1:C:194:PHE:CE1	1:D:251:MET:HB2	2.42	0.55
1:A:222:ALA:O	1:A:226:LEU:HB2	2.07	0.55
1:B:222:ALA:O	1:B:226:LEU:HB2	2.08	0.54
1:C:257:ILE:O	1:C:261:ILE:HG12	2.06	0.54
1:C:118:TYR:CD1	1:C:245:LEU:HD11	2.41	0.54
1:C:222:ALA:O	1:C:226:LEU:HB2	2.08	0.54
1:E:257:ILE:O	1:E:261:ILE:HG12	2.07	0.54
1:A:160:ASP:HB2	1:A:192:GLN:NE2	2.22	0.54
1:D:77:PHE:H	1:D:84:ARG:HD3	1.73	0.54
1:A:81:GLU:HG3	1:A:108:ARG:HG3	1.90	0.53
1:D:75:ILE:HD13	1:D:131:VAL:HB	1.89	0.53
1:E:149:GLY:HA3	1:E:164:PHE:HD2	1.73	0.53
1:D:213:THR:HG22	1:D:226:LEU:HD11	1.89	0.53
1:E:222:ALA:O	1:E:226:LEU:HB2	2.09	0.53
1:D:140:VAL:HG22	1:D:181:SER:HB3	1.89	0.53
1:E:160:ASP:HB2	1:E:192:GLN:NE2	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:LEU:N	1:A:149:GLY:O	2.41	0.53
1:B:248:THR:HG22	1:B:249:PRO:HD2	1.90	0.53
1:E:23:LEU:N	1:E:149:GLY:O	2.41	0.53
1:D:149:GLY:HA3	1:D:164:PHE:HD2	1.73	0.52
1:B:118:TYR:CD1	1:B:245:LEU:HD11	2.45	0.52
1:E:213:THR:HG22	1:E:226:LEU:HD11	1.91	0.52
1:A:118:TYR:CD1	1:A:245:LEU:HD11	2.44	0.52
1:E:248:THR:HG22	1:E:249:PRO:HD2	1.92	0.52
1:B:160:ASP:HB2	1:B:192:GLN:NE2	2.25	0.52
1:C:212:TRP:HB2	1:C:215:PHE:CE2	2.44	0.52
1:C:207:ILE:HG22	1:D:231:LEU:HD21	1.90	0.52
1:D:24:ILE:HD13	1:D:104:ARG:HE	1.74	0.52
1:E:195:SER:HB2	1:E:199:ASN:ND2	2.25	0.51
1:B:35:THR:OG1	1:B:108:ARG:NH2	2.42	0.51
1:A:248:THR:HG22	1:A:249:PRO:HD2	1.92	0.51
1:D:222:ALA:O	1:D:226:LEU:HB2	2.11	0.51
1:A:231:LEU:HD21	1:E:207:ILE:HG22	1.93	0.51
1:A:122:SER:HA	1:A:190:SER:HA	1.92	0.51
1:C:35:THR:OG1	1:C:108:ARG:NH2	2.43	0.51
1:E:81:GLU:HG3	1:E:108:ARG:HG3	1.92	0.51
1:A:61:ARG:HG2	1:A:62:VAL:HG23	1.92	0.51
1:A:140:VAL:HG22	1:A:181:SER:HB3	1.93	0.51
1:B:140:VAL:HG22	1:B:181:SER:HB3	1.93	0.51
1:D:160:ASP:HB2	1:D:192:GLN:NE2	2.26	0.51
1:C:197:ILE:HB	1:C:198:PRO:HD3	1.93	0.50
1:C:212:TRP:HZ3	1:C:264:PHE:HD2	1.59	0.50
1:D:248:THR:HG22	1:D:249:PRO:HD2	1.93	0.50
1:C:55:PRO:HG3	1:C:95:PRO:HB3	1.92	0.50
1:C:149:GLY:HA3	1:C:164:PHE:HD2	1.76	0.50
1:C:160:ASP:HB2	1:C:192:GLN:NE2	2.27	0.50
1:B:75:ILE:HD13	1:B:131:VAL:HB	1.94	0.50
1:C:203:PRO:HB2	1:C:237:PHE:CZ	2.47	0.50
1:C:257:ILE:HG22	1:C:309:LEU:HD23	1.94	0.49
1:C:195:SER:HB2	1:C:199:ASN:ND2	2.27	0.49
1:C:248:THR:HG22	1:C:249:PRO:HD2	1.94	0.49
1:D:35:THR:OG1	1:D:108:ARG:NH2	2.43	0.49
1:E:197:ILE:HB	1:E:198:PRO:HD3	1.94	0.49
1:A:267:VAL:HA	1:A:270:ILE:HB	1.95	0.49
1:D:147:LYS:HE2	1:D:165:THR:HA	1.95	0.49
1:B:197:ILE:HB	1:B:198:PRO:HD3	1.94	0.49
1:B:237:PHE:HB2	1:C:235:ILE:HD13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:268:ALA:O	1:C:272:VAL:HG13	2.13	0.48
1:E:149:GLY:HA3	1:E:164:PHE:CD2	2.48	0.48
1:A:77:PHE:O	1:E:104:ARG:NH1	2.40	0.48
1:B:278:LEU:HB3	1:B:287:ALA:HB2	1.95	0.48
1:D:149:GLY:HA3	1:D:164:PHE:CD2	2.49	0.48
1:E:75:ILE:HD13	1:E:131:VAL:HB	1.96	0.48
1:D:118:TYR:CD1	1:D:245:LEU:HD11	2.48	0.48
1:C:61:ARG:HG2	1:C:62:VAL:HG23	1.95	0.48
1:E:118:TYR:CE1	1:E:245:LEU:HD21	2.49	0.48
1:C:140:VAL:HG22	1:C:181:SER:HB3	1.95	0.48
1:D:195:SER:HB2	1:D:199:ASN:ND2	2.28	0.48
1:D:212:TRP:HZ3	1:D:264:PHE:HD2	1.62	0.48
1:A:118:TYR:CE1	1:A:245:LEU:HD21	2.48	0.48
1:E:7:PRO:C	1:E:50:ARG:HH12	2.23	0.47
1:E:212:TRP:HZ3	1:E:264:PHE:HD2	1.62	0.47
1:B:149:GLY:HA3	1:B:164:PHE:HD2	1.80	0.47
1:C:267:VAL:HA	1:C:270:ILE:HB	1.95	0.47
1:D:197:ILE:HB	1:D:198:PRO:HD3	1.95	0.47
1:E:218:THR:HG22	1:E:279:LYS:HE2	1.97	0.47
1:A:9:PRO:HD3	1:A:71:TRP:CE3	2.50	0.47
1:D:133:SER:HB2	1:D:137:ARG:HH11	1.78	0.47
1:E:61:ARG:HG2	1:E:62:VAL:HG23	1.95	0.47
1:A:197:ILE:HB	1:A:198:PRO:HD3	1.96	0.47
1:E:130:ILE:HA	1:E:181:SER:O	2.14	0.47
1:D:267:VAL:HA	1:D:270:ILE:HB	1.97	0.47
1:B:133:SER:HB2	1:B:137:ARG:HH11	1.80	0.46
1:D:18:ASN:O	1:D:44:LEU:HA	2.15	0.46
1:C:22:TYR:HB3	1:C:41:PHE:HB2	1.96	0.46
1:E:212:TRP:HB2	1:E:215:PHE:CE2	2.50	0.46
1:A:133:SER:HB2	1:A:137:ARG:HH11	1.80	0.46
1:B:24:ILE:HD13	1:B:104:ARG:HE	1.80	0.46
1:C:37:LYS:HG3	1:C:108:ARG:HB3	1.97	0.46
1:A:278:LEU:HB3	1:A:287:ALA:HB2	1.98	0.46
1:D:257:ILE:HG22	1:D:309:LEU:HD23	1.97	0.46
1:B:195:SER:HB2	1:B:199:ASN:ND2	2.31	0.46
1:C:149:GLY:HA3	1:C:164:PHE:CD2	2.51	0.46
1:B:149:GLY:HA3	1:B:164:PHE:CD2	2.51	0.45
1:C:213:THR:HG22	1:C:226:LEU:HD11	1.97	0.45
1:A:195:SER:HB2	1:A:199:ASN:ND2	2.31	0.45
1:A:104:ARG:HD2	1:B:76:ARG:NH1	2.32	0.45
1:A:132:ARG:HA	1:A:180:GLU:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:9:PRO:HD3	1:E:71:TRP:CE3	2.52	0.45
1:C:118:TYR:CE1	1:C:245:LEU:HD21	2.51	0.45
1:D:212:TRP:HB2	1:D:215:PHE:CE2	2.51	0.45
1:E:9:PRO:HB3	1:E:48:ASP:CG	2.41	0.45
1:E:133:SER:HB2	1:E:137:ARG:HH11	1.81	0.45
1:D:118:TYR:CE1	1:D:245:LEU:HD21	2.52	0.45
1:C:9:PRO:HD3	1:C:71:TRP:CE3	2.52	0.45
1:D:194:PHE:CD1	1:D:194:PHE:C	2.94	0.45
1:A:268:ALA:O	1:A:272:VAL:HG13	2.17	0.45
1:B:212:TRP:HB2	1:B:215:PHE:CE2	2.52	0.45
1:B:194:PHE:CD1	1:B:194:PHE:C	2.95	0.45
1:D:25:GLU:HB2	1:D:39:ASN:HB3	1.98	0.45
1:D:61:ARG:HG2	1:D:62:VAL:HG23	1.99	0.45
1:E:194:PHE:C	1:E:194:PHE:CD1	2.94	0.45
1:A:7:PRO:C	1:A:50:ARG:HH12	2.25	0.44
1:C:194:PHE:CD1	1:C:194:PHE:C	2.95	0.44
1:E:308:ILE:O	1:E:312:LEU:HB2	2.17	0.44
1:A:9:PRO:HB3	1:A:48:ASP:CG	2.42	0.44
1:A:212:TRP:HB2	1:A:215:PHE:CE2	2.53	0.44
1:C:207:ILE:HG13	1:C:208:LEU:N	2.33	0.44
1:D:27:TYR:HB3	1:E:110:LEU:HD11	1.99	0.44
1:D:115:PHE:CG	1:D:245:LEU:HD13	2.53	0.44
1:D:226:LEU:HD22	1:D:226:LEU:HA	1.80	0.44
1:C:283:GLN:N	1:C:284:PRO:HD3	2.33	0.44
1:E:8:PRO:O	1:E:50:ARG:NH1	2.50	0.44
1:A:194:PHE:CD1	1:A:194:PHE:C	2.94	0.44
1:C:15:LEU:HD11	1:C:46:TRP:HB2	1.99	0.44
1:B:267:VAL:HA	1:B:270:ILE:HB	1.99	0.44
1:E:252:THR:OG1	1:E:253:TYR:N	2.51	0.44
1:C:147:LYS:HE2	1:C:165:THR:HA	2.00	0.44
1:D:52:ALA:HB1	1:D:95:PRO:O	2.18	0.44
1:A:18:ASN:HB2	1:A:45:SER:OG	2.17	0.44
1:A:212:TRP:HZ3	1:A:264:PHE:HD2	1.65	0.44
1:A:104:ARG:HD2	1:B:76:ARG:HH11	1.82	0.43
1:B:132:ARG:HA	1:B:180:GLU:HG2	2.00	0.43
1:B:305:ALA:O	1:B:309:LEU:HB2	2.17	0.43
1:D:9:PRO:HB3	1:D:48:ASP:CG	2.43	0.43
1:A:77:PHE:CG	1:A:84:ARG:HD2	2.54	0.43
1:A:283:GLN:N	1:A:284:PRO:HD3	2.32	0.43
1:B:9:PRO:HB3	1:B:48:ASP:CG	2.43	0.43
1:E:305:ALA:O	1:E:309:LEU:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:GLN:N	1:B:284:PRO:HD3	2.33	0.43
1:B:252:THR:OG1	1:B:253:TYR:N	2.50	0.43
1:D:13:GLU:HB3	1:D:14:PRO:HD2	2.00	0.43
1:D:207:ILE:HG13	1:D:208:LEU:N	2.33	0.43
1:A:252:THR:OG1	1:A:253:TYR:N	2.52	0.43
1:D:42:LEU:HB3	1:D:103:GLU:CG	2.47	0.43
1:A:36:PHE:CE1	1:A:109:VAL:HB	2.54	0.43
1:A:207:ILE:HG22	1:B:231:LEU:HD21	2.00	0.43
1:B:268:ALA:O	1:B:272:VAL:HG13	2.18	0.43
1:D:227:VAL:HG11	1:D:269:VAL:HG23	2.01	0.43
1:E:18:ASN:O	1:E:44:LEU:HA	2.18	0.43
1:A:183:LEU:HD23	1:A:183:LEU:HA	1.87	0.43
1:B:37:LYS:HG3	1:B:108:ARG:HB3	2.00	0.43
1:E:22:TYR:HB3	1:E:41:PHE:HB2	2.00	0.43
1:E:122:SER:HA	1:E:190:SER:HA	2.00	0.43
1:E:207:ILE:HG13	1:E:208:LEU:N	2.34	0.43
1:D:77:PHE:CG	1:D:84:ARG:HD2	2.54	0.43
1:E:183:LEU:HD23	1:E:183:LEU:HA	1.83	0.43
1:A:149:GLY:HA3	1:A:164:PHE:HD2	1.85	0.42
1:D:124:THR:O	1:D:124:THR:OG1	2.34	0.42
1:D:94:SER:HB3	1:D:98:THR:HB	2.01	0.42
1:A:75:ILE:HD13	1:A:131:VAL:HB	2.01	0.42
1:D:21:ILE:HA	1:D:41:PHE:O	2.20	0.42
1:D:283:GLN:N	1:D:284:PRO:HD3	2.34	0.42
1:E:51:LEU:HD13	1:E:70:ILE:HD12	2.01	0.42
1:A:203:PRO:HB2	1:A:237:PHE:CZ	2.55	0.42
1:B:18:ASN:O	1:B:44:LEU:HA	2.20	0.42
1:A:24:ILE:HD13	1:A:104:ARG:HE	1.85	0.42
1:A:237:PHE:HB2	1:B:235:ILE:HD13	2.00	0.42
1:B:155:PHE:CE1	1:C:110:LEU:HD21	2.54	0.42
1:B:13:GLU:HB3	1:B:14:PRO:HD2	2.02	0.42
1:C:133:SER:HB2	1:C:137:ARG:HH11	1.85	0.42
1:A:29:LEU:HD23	1:A:159:TRP:NE1	2.35	0.42
1:C:34:GLU:HB3	1:C:113:LEU:HG	2.02	0.41
1:C:234:HIS:CE1	1:C:261:ILE:HG21	2.55	0.41
1:E:247:LYS:O	1:E:247:LYS:HG3	2.19	0.41
1:B:226:LEU:HD22	1:B:226:LEU:HA	1.82	0.41
1:C:252:THR:OG1	1:C:253:TYR:N	2.52	0.41
1:D:130:ILE:HA	1:D:181:SER:O	2.20	0.41
1:D:132:ARG:HA	1:D:180:GLU:HG2	2.02	0.41
1:A:130:ILE:HA	1:A:181:SER:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:LEU:HD12	1:A:309:LEU:HA	1.89	0.41
1:B:207:ILE:HG13	1:B:208:LEU:N	2.33	0.41
1:B:218:THR:HG22	1:B:279:LYS:HE2	2.02	0.41
1:D:36:PHE:CE1	1:D:109:VAL:HB	2.55	0.41
1:D:252:THR:OG1	1:D:253:TYR:N	2.54	0.41
1:E:7:PRO:O	1:E:50:ARG:NH1	2.49	0.41
1:E:278:LEU:HD12	1:E:278:LEU:HA	1.87	0.41
1:A:28:SER:O	1:A:36:PHE:HA	2.21	0.41
1:A:207:ILE:HG13	1:A:208:LEU:N	2.35	0.41
1:B:124:THR:O	1:B:124:THR:OG1	2.37	0.41
1:C:36:PHE:CE1	1:C:109:VAL:HB	2.55	0.41
1:C:132:ARG:HA	1:C:180:GLU:HG2	2.03	0.41
1:D:268:ALA:O	1:D:272:VAL:HG13	2.20	0.41
1:E:268:ALA:O	1:E:272:VAL:HG13	2.21	0.41
1:B:27:TYR:HB3	1:C:110:LEU:HD11	2.02	0.41
1:B:81:GLU:OE2	1:B:110:LEU:HD12	2.21	0.41
1:C:104:ARG:HD2	1:D:76:ARG:HH11	1.85	0.41
1:A:77:PHE:HD2	1:A:80:VAL:HG21	1.85	0.41
1:B:212:TRP:HZ3	1:B:264:PHE:HD2	1.69	0.41
1:C:115:PHE:CG	1:C:245:LEU:HD13	2.56	0.41
1:C:135:ASP:CG	1:C:136:THR:N	2.79	0.41
1:C:305:ALA:O	1:C:309:LEU:HB2	2.21	0.41
1:E:283:GLN:N	1:E:284:PRO:HD3	2.35	0.41
1:A:147:LYS:O	1:A:147:LYS:HG2	2.21	0.41
1:B:130:ILE:HA	1:B:181:SER:O	2.21	0.41
1:D:203:PRO:HB2	1:D:237:PHE:CZ	2.55	0.41
1:B:247:LYS:O	1:B:247:LYS:HG3	2.20	0.40
1:A:225:THR:O	1:A:229:SER:HB2	2.21	0.40
1:C:125:LEU:HD12	1:C:187:LEU:HD23	2.03	0.40
1:C:218:THR:HG22	1:C:279:LYS:HE2	2.03	0.40
1:D:23:LEU:HD13	1:D:26:CYS:SG	2.61	0.40
1:E:42:LEU:HB3	1:E:103:GLU:CG	2.51	0.40
1:E:318:PHE:C	1:E:320:PHE:H	2.29	0.40
1:B:309:LEU:HD12	1:B:309:LEU:HA	1.92	0.40
1:C:13:GLU:HB3	1:C:14:PRO:HD2	2.03	0.40
1:D:81:GLU:OE2	1:D:110:LEU:HD12	2.22	0.40
1:A:149:GLY:HA3	1:A:164:PHE:CD2	2.57	0.40
1:C:147:LYS:O	1:C:147:LYS:HG2	2.21	0.40
1:D:200:ILE:HD12	1:D:241:VAL:HG11	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	308/316 (98%)	282 (92%)	25 (8%)	1 (0%)	36	67
1	B	308/316 (98%)	282 (92%)	25 (8%)	1 (0%)	36	67
1	C	308/316 (98%)	285 (92%)	22 (7%)	1 (0%)	36	67
1	D	308/316 (98%)	282 (92%)	25 (8%)	1 (0%)	36	67
1	E	308/316 (98%)	282 (92%)	25 (8%)	1 (0%)	36	67
All	All	1540/1580 (98%)	1413 (92%)	122 (8%)	5 (0%)	36	67

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	148	VAL
1	B	148	VAL
1	C	148	VAL
1	D	148	VAL
1	E	148	VAL

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	277/283 (98%)	251 (91%)	26 (9%)	8	31
1	B	277/283 (98%)	249 (90%)	28 (10%)	7	29
1	C	277/283 (98%)	253 (91%)	24 (9%)	9	35
1	D	277/283 (98%)	251 (91%)	26 (9%)	8	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	277/283 (98%)	250 (90%)	27 (10%)	8	31
All	All	1385/1415 (98%)	1254 (90%)	131 (10%)	8	31

All (131) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	THR
1	A	54	ASP
1	A	84	ARG
1	A	109	VAL
1	A	120	PHE
1	A	124	THR
1	A	135	ASP
1	A	140	VAL
1	A	147	LYS
1	A	156	LEU
1	A	157	THR
1	A	162	GLU
1	A	179	LEU
1	A	200	ILE
1	A	213	THR
1	A	221	GLU
1	A	226	LEU
1	A	245	LEU
1	A	247	LYS
1	A	248	THR
1	A	252	THR
1	A	254	THR
1	A	263	LEU
1	A	272	VAL
1	A	278	LEU
1	A	303	LEU
1	B	16	THR
1	B	54	ASP
1	B	84	ARG
1	B	109	VAL
1	B	120	PHE
1	B	124	THR
1	B	135	ASP
1	B	138	ASN
1	B	140	VAL
1	B	141	LEU

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Mol	Chain	Res	Type
1	B	147	LYS
1	B	156	LEU
1	B	162	GLU
1	B	179	LEU
1	B	200	ILE
1	B	213	THR
1	B	221	GLU
1	B	226	LEU
1	B	245	LEU
1	B	247	LYS
1	B	248	THR
1	B	252	THR
1	B	254	THR
1	B	263	LEU
1	B	269	VAL
1	B	278	LEU
1	B	303	LEU
1	B	309	LEU
1	C	54	ASP
1	C	84	ARG
1	C	109	VAL
1	C	120	PHE
1	C	124	THR
1	C	135	ASP
1	C	138	ASN
1	C	140	VAL
1	C	156	LEU
1	C	157	THR
1	C	162	GLU
1	C	179	LEU
1	C	200	ILE
1	C	213	THR
1	C	221	GLU
1	C	226	LEU
1	C	245	LEU
1	C	247	LYS
1	C	248	THR
1	C	252	THR
1	C	254	THR
1	C	263	LEU
1	C	278	LEU
1	C	303	LEU

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Mol	Chain	Res	Type
1	D	54	ASP
1	D	84	ARG
1	D	109	VAL
1	D	120	PHE
1	D	124	THR
1	D	135	ASP
1	D	140	VAL
1	D	147	LYS
1	D	156	LEU
1	D	157	THR
1	D	162	GLU
1	D	179	LEU
1	D	200	ILE
1	D	213	THR
1	D	221	GLU
1	D	226	LEU
1	D	245	LEU
1	D	247	LYS
1	D	248	THR
1	D	252	THR
1	D	254	THR
1	D	263	LEU
1	D	269	VAL
1	D	278	LEU
1	D	303	LEU
1	D	309	LEU
1	E	54	ASP
1	E	84	ARG
1	E	109	VAL
1	E	124	THR
1	E	135	ASP
1	E	138	ASN
1	E	140	VAL
1	E	141	LEU
1	E	147	LYS
1	E	156	LEU
1	E	157	THR
1	E	162	GLU
1	E	179	LEU
1	E	200	ILE
1	E	213	THR
1	E	221	GLU

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Mol	Chain	Res	Type
1	E	226	LEU
1	E	245	LEU
1	E	247	LYS
1	E	248	THR
1	E	252	THR
1	E	254	THR
1	E	263	LEU
1	E	272	VAL
1	E	278	LEU
1	E	303	LEU
1	E	309	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	ASN
1	A	234	HIS
1	A	283	GLN
1	B	283	GLN
1	C	126	HIS
1	C	234	HIS
1	D	39	ASN
1	E	234	HIS
1	E	306	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 oligosaccharides 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, 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	310/316 (98%)	1.08	64 (20%) 2 2	59, 95, 161, 240	0
1	B	310/316 (98%)	1.11	65 (20%) 2 2	63, 96, 155, 239	0
1	C	310/316 (98%)	0.91	47 (15%) 5 4	56, 92, 145, 204	0
1	D	310/316 (98%)	1.12	58 (18%) 3 3	59, 92, 137, 177	0
1	E	310/316 (98%)	0.93	47 (15%) 5 4	61, 90, 147, 228	0
All	All	1550/1580 (98%)	1.03	281 (18%) 3 3	56, 93, 151, 240	0

All (281) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	90	ASP	8.8
1	B	148	VAL	8.1
1	E	144	ASP	7.6
1	B	144	ASP	7.5
1	B	7	PRO	7.1
1	E	148	VAL	6.8
1	C	59	GLY	6.3
1	A	7	PRO	6.1
1	C	74	GLU	5.8
1	C	173	PHE	5.8
1	A	148	VAL	5.6
1	D	148	VAL	5.6
1	C	7	PRO	5.5
1	B	18	ASN	5.4
1	E	59	GLY	5.3
1	E	7	PRO	5.2
1	A	173	PHE	5.2
1	D	45	SER	5.1
1	A	60	VAL	5.0
1	B	244	ASN	4.9

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Mol	Chain	Res	Type	RSRZ
1	D	100	GLN	4.8
1	B	54	ASP	4.8
1	D	144	ASP	4.8
1	A	65	TYR	4.7
1	B	138	ASN	4.7
1	C	60	VAL	4.7
1	B	58	SER	4.7
1	C	194	PHE	4.7
1	A	59	GLY	4.6
1	D	7	PRO	4.5
1	B	194	PHE	4.5
1	A	145	LEU	4.5
1	D	194	PHE	4.5
1	A	244	ASN	4.4
1	B	173	PHE	4.3
1	D	173	PHE	4.3
1	D	90	ASP	4.3
1	A	74	GLU	4.3
1	D	11	ALA	4.3
1	D	136	THR	4.2
1	D	114	ASP	4.1
1	C	144	ASP	4.1
1	B	246	GLY	4.1
1	B	243	THR	4.1
1	E	173	PHE	4.1
1	B	145	LEU	4.1
1	C	247	LYS	3.9
1	E	136	THR	3.9
1	E	194	PHE	3.9
1	A	136	THR	3.8
1	A	207	ILE	3.8
1	A	141	LEU	3.8
1	A	243	THR	3.8
1	A	194	PHE	3.7
1	A	63	LYS	3.7
1	D	64	THR	3.7
1	D	10	ILE	3.7
1	A	11	ALA	3.6
1	A	144	ASP	3.6
1	D	101	TYR	3.6
1	A	101	TYR	3.6
1	A	88	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	13	GLU	3.6
1	B	59	GLY	3.6
1	A	53	PHE	3.5
1	A	316	PHE	3.5
1	C	138	ASN	3.5
1	B	100	GLN	3.5
1	E	143	VAL	3.5
1	E	244	ASN	3.5
1	E	246	GLY	3.5
1	A	90	ASP	3.5
1	D	188	ARG	3.5
1	B	193	TYR	3.4
1	E	60	VAL	3.4
1	C	177	ASP	3.4
1	A	64	THR	3.4
1	D	207	ILE	3.4
1	A	67	PRO	3.4
1	B	89	VAL	3.4
1	E	57	ARG	3.4
1	D	66	GLU	3.3
1	B	136	THR	3.3
1	D	71	TRP	3.3
1	E	47	LYS	3.3
1	B	134	VAL	3.2
1	A	138	ASN	3.2
1	D	57	ARG	3.2
1	B	83	ALA	3.2
1	C	246	GLY	3.2
1	B	143	VAL	3.2
1	D	92	SER	3.2
1	E	193	TYR	3.2
1	B	192	GLN	3.2
1	B	142	ALA	3.2
1	C	71	TRP	3.2
1	A	176	GLU	3.2
1	D	143	VAL	3.2
1	E	55	PRO	3.2
1	A	54	ASP	3.1
1	D	138	ASN	3.1
1	B	92	SER	3.1
1	B	135	ASP	3.1
1	D	196	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	288	ALA	3.1
1	B	60	VAL	3.1
1	E	10	ILE	3.1
1	A	142	ALA	3.0
1	E	176	GLU	3.0
1	A	137	ARG	3.0
1	B	177	ASP	3.0
1	D	26	CYS	3.0
1	D	60	VAL	2.9
1	A	55	PRO	2.9
1	B	11	ALA	2.9
1	B	45	SER	2.9
1	B	47	LYS	2.9
1	A	87	ASP	2.9
1	C	14	PRO	2.9
1	E	146	GLU	2.9
1	A	282	SER	2.9
1	D	244	ASN	2.9
1	B	247	LYS	2.9
1	D	72	ILE	2.9
1	D	56	VAL	2.8
1	C	207	ILE	2.8
1	D	211	SER	2.8
1	D	282	SER	2.8
1	C	243	THR	2.8
1	E	212	TRP	2.8
1	D	47	LYS	2.8
1	E	56	VAL	2.8
1	C	66	GLU	2.8
1	A	212	TRP	2.7
1	B	57	ARG	2.7
1	A	192	GLN	2.7
1	C	143	VAL	2.7
1	A	13	GLU	2.7
1	B	114	ASP	2.7
1	A	247	LYS	2.7
1	A	12	ASP	2.7
1	E	54	ASP	2.7
1	E	18	ASN	2.7
1	A	245	LEU	2.7
1	B	64	THR	2.7
1	D	98	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	139	ILE	2.7
1	A	246	GLY	2.7
1	B	245	LEU	2.7
1	E	76	ARG	2.6
1	A	211	SER	2.6
1	B	101	TYR	2.6
1	B	12	ASP	2.6
1	D	87	ASP	2.6
1	C	55	PRO	2.6
1	D	76	ARG	2.6
1	D	192	GLN	2.6
1	B	176	GLU	2.6
1	C	136	THR	2.6
1	B	320	PHE	2.6
1	A	252	THR	2.6
1	C	141	LEU	2.6
1	D	46	TRP	2.6
1	B	76	ARG	2.6
1	A	95	PRO	2.6
1	E	138	ASN	2.6
1	C	193	TYR	2.6
1	D	12	ASP	2.6
1	A	76	ARG	2.6
1	B	56	VAL	2.6
1	E	147	LYS	2.6
1	C	72	ILE	2.5
1	C	148	VAL	2.5
1	D	247	LYS	2.5
1	A	10	ILE	2.5
1	D	212	TRP	2.5
1	A	114	ASP	2.5
1	B	196	TYR	2.5
1	A	147	LYS	2.5
1	C	192	GLN	2.5
1	B	49	ARG	2.5
1	D	88	VAL	2.5
1	D	83	ALA	2.5
1	B	10	ILE	2.5
1	C	54	ASP	2.5
1	B	216	TRP	2.5
1	C	145	LEU	2.5
1	A	196	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	282	SER	2.4
1	E	45	SER	2.4
1	C	61	ARG	2.4
1	E	196	TYR	2.4
1	C	134	VAL	2.4
1	D	283	GLN	2.4
1	C	282	SER	2.4
1	E	116	ARG	2.4
1	E	134	VAL	2.4
1	B	214	ALA	2.4
1	B	146	GLU	2.4
1	A	58	SER	2.4
1	A	9	PRO	2.4
1	A	56	VAL	2.4
1	E	177	ASP	2.4
1	C	10	ILE	2.4
1	E	58	SER	2.4
1	E	247	LYS	2.4
1	D	251	MET	2.4
1	A	70	ILE	2.3
1	E	135	ASP	2.3
1	E	320	PHE	2.3
1	C	95	PRO	2.3
1	D	67	PRO	2.3
1	C	252	THR	2.3
1	D	97	GLY	2.3
1	C	18	ASN	2.3
1	D	135	ASP	2.3
1	A	83	ALA	2.3
1	A	216	TRP	2.3
1	B	212	TRP	2.3
1	D	288	ALA	2.3
1	D	126	HIS	2.3
1	E	145	LEU	2.3
1	A	49	ARG	2.3
1	B	61	ARG	2.3
1	E	207	ILE	2.3
1	A	89	VAL	2.3
1	D	59	GLY	2.2
1	E	142	ALA	2.2
1	B	98	THR	2.2
1	C	65	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	169	LYS	2.2
1	C	254	THR	2.2
1	D	63	LYS	2.2
1	E	61	ARG	2.2
1	C	56	VAL	2.2
1	D	134	VAL	2.2
1	C	221	GLU	2.2
1	E	13	GLU	2.2
1	C	285	ALA	2.2
1	E	141	LEU	2.2
1	B	118	TYR	2.2
1	B	139	ILE	2.2
1	B	207	ILE	2.2
1	A	149	GLY	2.2
1	C	319	GLY	2.2
1	D	169	LYS	2.2
1	E	243	THR	2.2
1	B	140	VAL	2.2
1	B	319	GLY	2.2
1	D	243	THR	2.1
1	C	211	SER	2.1
1	A	281	GLU	2.1
1	C	292	ARG	2.1
1	D	68	GLU	2.1
1	C	153	ASP	2.1
1	A	143	VAL	2.1
1	B	91	ILE	2.1
1	C	196	TYR	2.1
1	E	245	LEU	2.1
1	C	11	ALA	2.1
1	A	72	ILE	2.1
1	E	65	TYR	2.1
1	B	74	GLU	2.1
1	A	96	ASP	2.1
1	A	61	ARG	2.1
1	D	146	GLU	2.1
1	B	169	LYS	2.1
1	A	135	ASP	2.1
1	E	114	ASP	2.1
1	E	68	GLU	2.1
1	B	84	ARG	2.0
1	D	231	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	177	ASP	2.0
1	B	147	LYS	2.0
1	D	176	GLU	2.0
1	B	122	SER	2.0
1	A	52	ALA	2.0
1	B	26	CYS	2.0
1	E	95	PRO	2.0
1	B	68	GLU	2.0
1	D	221	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 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.