



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 24, 2026 – 11:31 PM UTC

PDB ID : 5HEH / pdb_00005heh
Title : Pentameric ligand-gated ion channel GLIC mutant P246A
Authors : Bertozzi, C.; Dutzler, R.
Deposited on : 2016-01-06
Resolution : 3.30 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

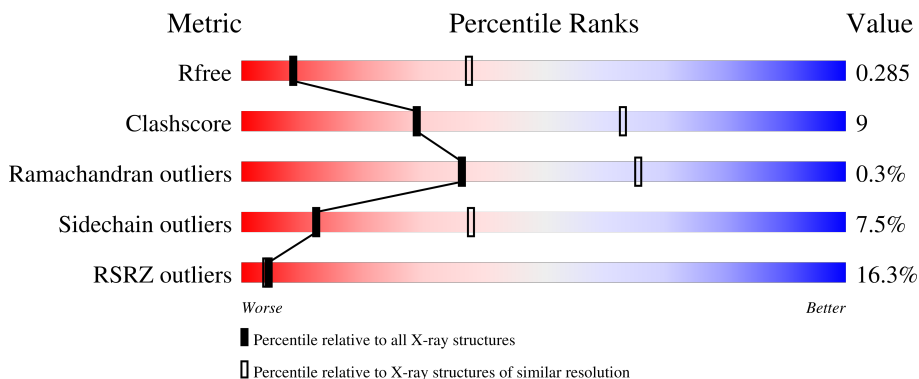
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	
1	B	316	
1	C	316	
1	D	316	
1	E	316	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12595 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
			2519	1660	403	452	4			
1	B	310	Total	C	N	O	S	0	0	0
			2519	1660	403	452	4			
1	C	310	Total	C	N	O	S	0	0	0
			2519	1660	403	452	4			
1	D	310	Total	C	N	O	S	0	0	0
			2519	1660	403	452	4			
1	E	310	Total	C	N	O	S	0	0	0
			2519	1660	403	452	4			

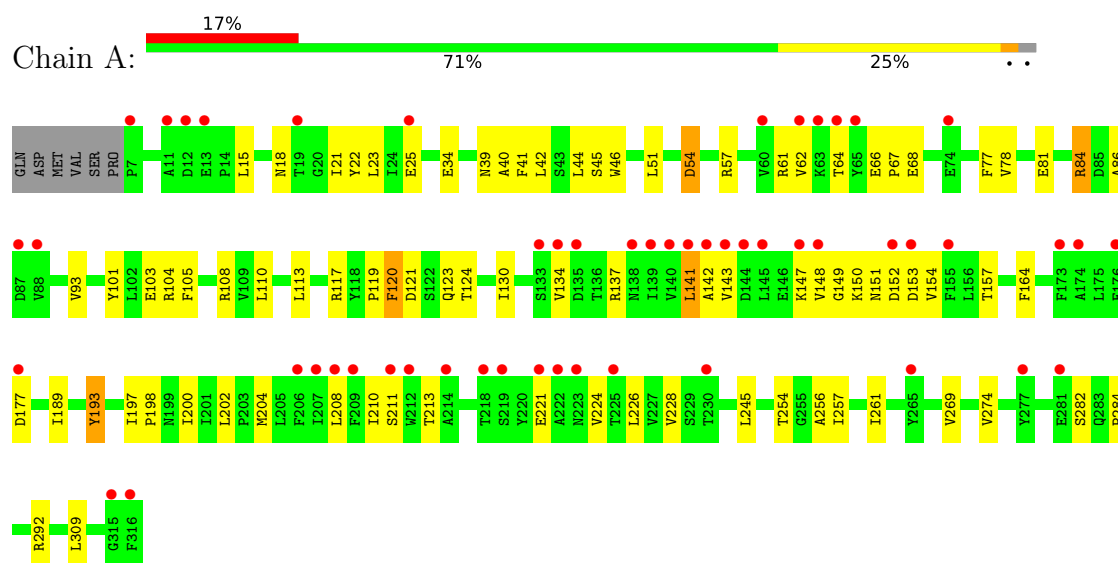
There are 5 discrepancies between the modelled and reference sequences:

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

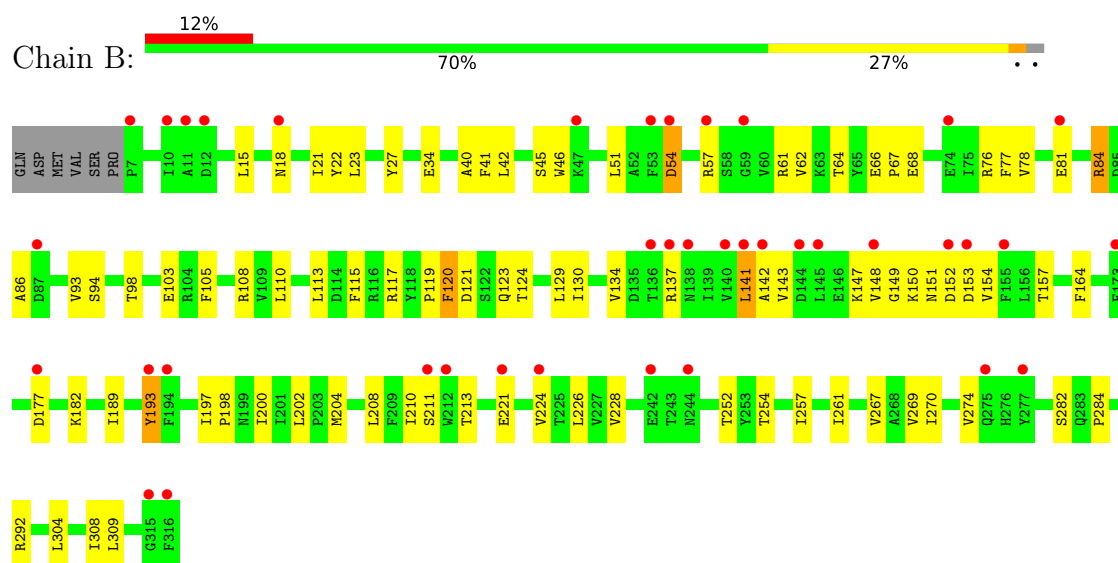
3 Residue-property plots

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.

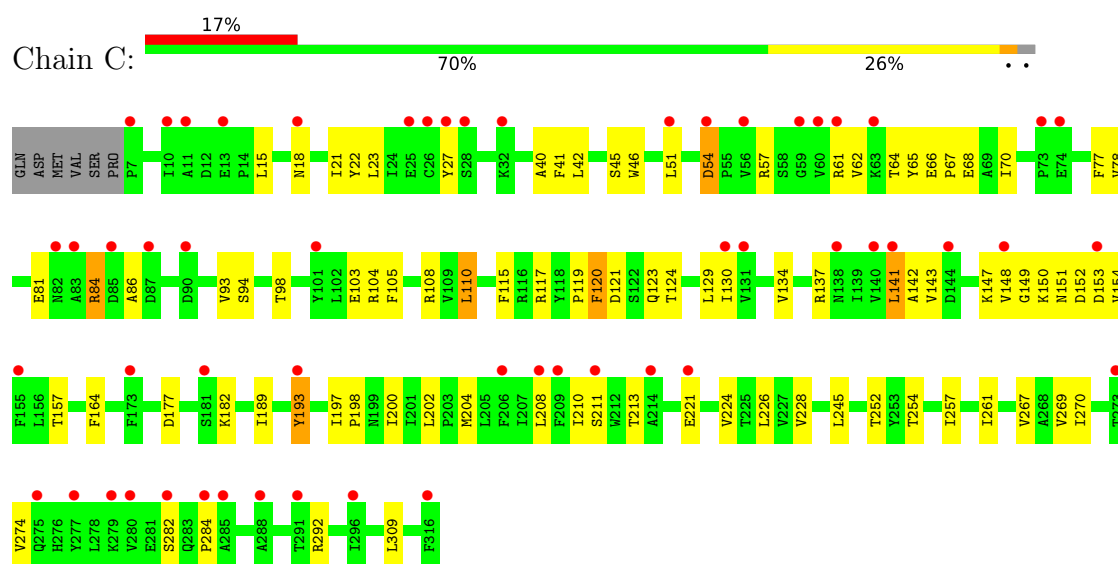
- Molecule 1: Proton-gated ion channel



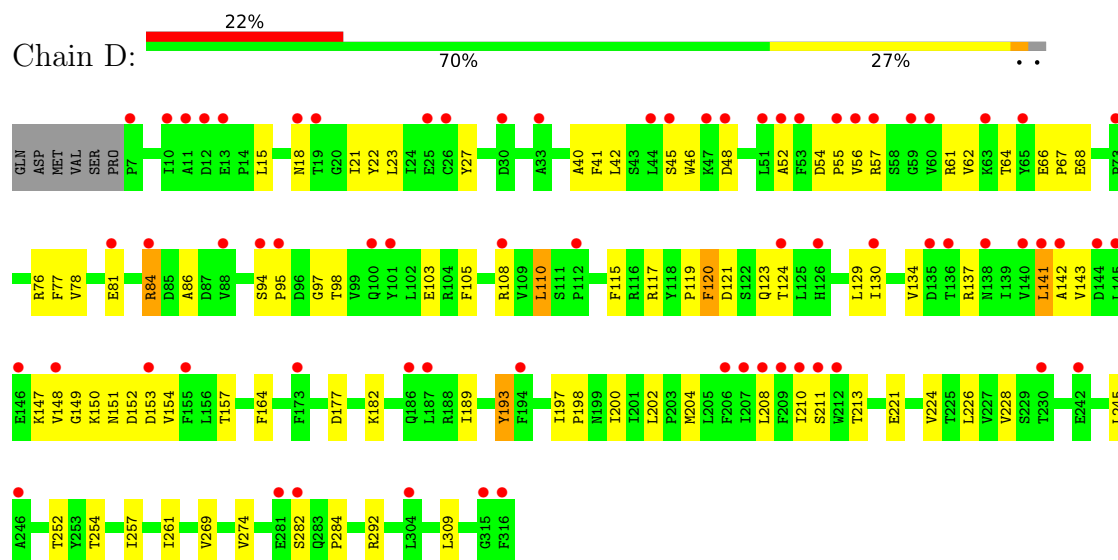
- Molecule 1: Proton-gated ion channel



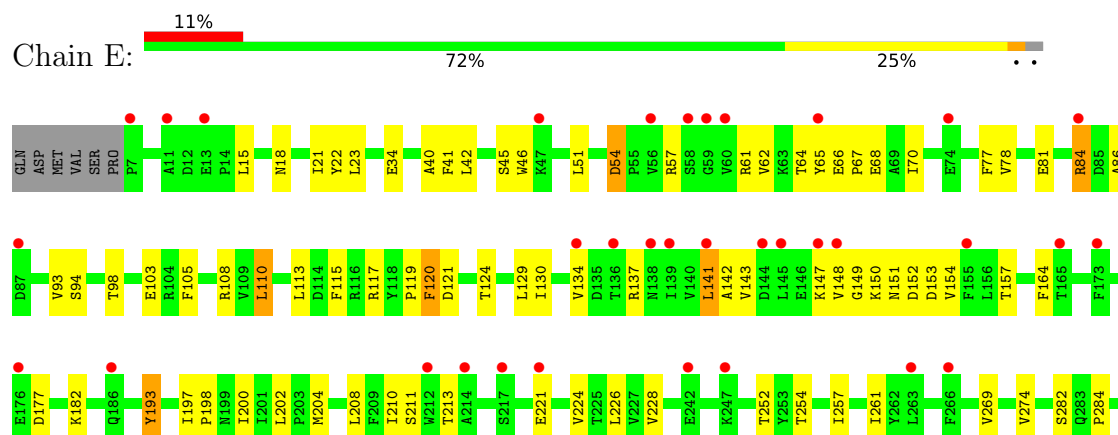
- Molecule 1: Proton-gated ion channel

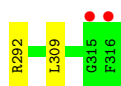


• Molecule 1: Proton-gated ion channel



• 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	177.69Å 133.94Å 159.83Å 90.00° 101.10° 90.00°	Depositor
Resolution (Å)	29.91 – 3.30 29.91 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.91-3.30) 99.4 (29.91-3.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 3.33Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.244 , 0.280 0.254 , 0.285	Depositor DCC
R_{free} test set	2798 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	87.8	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 60.5	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	0.89	EDS
Total number of atoms	12595	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% 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	0.13	0/2586	0.37	0/3530
1	B	0.13	0/2586	0.38	0/3530
1	C	0.13	0/2586	0.37	0/3530
1	D	0.14	0/2586	0.39	0/3530
1	E	0.13	0/2586	0.38	0/3530
All	All	0.13	0/12930	0.38	0/17650

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	2519	0	2535	45	0
1	B	2519	0	2535	47	0
1	C	2519	0	2535	48	0
1	D	2519	0	2535	50	0
1	E	2519	0	2535	42	0
All	All	12595	0	12675	220	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 9.

All (220) 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:C:22:TYR:HA	1:C:149:GLY:HA2	1.54	0.90
1:D:22:TYR:HA	1:D:149:GLY:HA2	1.54	0.88
1:B:22:TYR:HA	1:B:149:GLY:HA2	1.54	0.88
1:E:22:TYR:HA	1:E:149:GLY:HA2	1.53	0.86
1:A:22:TYR:HA	1:A:149:GLY:HA2	1.55	0.86
1:C:78:VAL:HG22	1:C:130:ILE:HG12	1.74	0.69
1:B:22:TYR:HB3	1:B:41:PHE:HB2	1.75	0.69
1:B:78:VAL:HG22	1:B:130:ILE:HG12	1.75	0.68
1:D:22:TYR:HB3	1:D:41:PHE:HB2	1.76	0.68
1:E:78:VAL:HG22	1:E:130:ILE:HG12	1.76	0.68
1:A:78:VAL:HG22	1:A:130:ILE:HG12	1.76	0.67
1:D:78:VAL:HG22	1:D:130:ILE:HG12	1.76	0.67
1:A:22:TYR:HB3	1:A:41:PHE:HB2	1.76	0.66
1:C:61:ARG:HG2	1:C:62:VAL:HG23	1.78	0.65
1:E:22:TYR:HB3	1:E:41:PHE:HB2	1.77	0.65
1:B:147:LYS:O	1:B:149:GLY:N	2.28	0.65
1:C:22:TYR:HB3	1:C:41:PHE:HB2	1.78	0.65
1:D:147:LYS:O	1:D:149:GLY:N	2.30	0.65
1:E:147:LYS:O	1:E:149:GLY:N	2.29	0.65
1:A:147:LYS:O	1:A:149:GLY:N	2.30	0.64
1:C:147:LYS:O	1:C:149:GLY:N	2.31	0.63
1:D:61:ARG:HG2	1:D:62:VAL:HG23	1.81	0.61
1:A:61:ARG:HG2	1:A:62:VAL:HG23	1.83	0.61
1:B:210:ILE:HG23	1:C:269:VAL:HG11	1.83	0.60
1:D:94:SER:HB3	1:D:98:THR:HB	1.83	0.60
1:B:61:ARG:HG2	1:B:62:VAL:HG23	1.85	0.59
1:A:282:SER:C	1:A:284:PRO:HD3	2.29	0.58
1:E:61:ARG:HG2	1:E:62:VAL:HG23	1.86	0.58
1:E:282:SER:C	1:E:284:PRO:HD3	2.28	0.58
1:A:210:ILE:HG23	1:B:269:VAL:HG11	1.85	0.57
1:C:282:SER:C	1:C:284:PRO:HD3	2.29	0.57
1:D:282:SER:C	1:D:284:PRO:HD3	2.29	0.57
1:E:81:GLU:HG3	1:E:108:ARG:HG3	1.86	0.56
1:A:42:LEU:HB3	1:A:103:GLU:HG2	1.88	0.56
1:A:269:VAL:HG11	1:E:210:ILE:HG23	1.88	0.56
1:D:42:LEU:HB3	1:D:103:GLU:HG2	1.86	0.56
1:B:282:SER:C	1:B:284:PRO:HD3	2.29	0.56
1:C:42:LEU:HB3	1:C:103:GLU:HG2	1.88	0.54
1:B:42:LEU:HB3	1:B:103:GLU:HG2	1.88	0.54
1:E:42:LEU:HB3	1:E:103:GLU:HG2	1.89	0.54
1:D:210:ILE:HG23	1:E:269:VAL:HG11	1.90	0.53
1:D:27:TYR:HB3	1:E:110:LEU:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:120:PHE:HD2	1:E:193:TYR:CD2	2.27	0.53
1:C:151:ASN:OD1	1:C:152:ASP:N	2.42	0.53
1:E:151:ASN:OD1	1:E:152:ASP:N	2.42	0.52
1:B:151:ASN:OD1	1:B:152:ASP:N	2.42	0.52
1:A:81:GLU:HG3	1:A:108:ARG:HG3	1.91	0.52
1:B:81:GLU:HG3	1:B:108:ARG:HG3	1.91	0.52
1:C:81:GLU:HG3	1:C:108:ARG:HG3	1.92	0.52
1:D:151:ASN:OD1	1:D:152:ASP:N	2.42	0.52
1:A:151:ASN:OD1	1:A:152:ASP:N	2.43	0.51
1:B:120:PHE:HD2	1:B:193:TYR:CD2	2.29	0.51
1:A:86:ALA:HA	1:A:105:PHE:HA	1.92	0.51
1:D:81:GLU:HG3	1:D:108:ARG:HG3	1.93	0.51
1:D:120:PHE:HD2	1:D:193:TYR:CD2	2.28	0.51
1:E:34:GLU:OE2	1:E:113:LEU:N	2.37	0.50
1:A:120:PHE:HD2	1:A:193:TYR:CD2	2.30	0.50
1:E:141:LEU:HD23	1:E:142:ALA:H	1.77	0.50
1:D:54:ASP:OD1	1:D:57:ARG:HB2	2.12	0.49
1:E:117:ARG:O	1:E:121:ASP:HB3	2.13	0.49
1:B:224:VAL:O	1:B:228:VAL:HB	2.13	0.48
1:C:120:PHE:HD2	1:C:193:TYR:CD2	2.30	0.48
1:C:200:ILE:O	1:C:204:MET:HB2	2.13	0.48
1:A:224:VAL:O	1:A:228:VAL:HB	2.13	0.48
1:D:208:LEU:HD13	1:D:261:ILE:HG23	1.96	0.48
1:B:117:ARG:O	1:B:121:ASP:HB3	2.14	0.48
1:C:151:ASN:O	1:C:154:VAL:HG22	2.14	0.48
1:A:200:ILE:O	1:A:204:MET:HB2	2.13	0.47
1:C:224:VAL:O	1:C:228:VAL:HB	2.14	0.47
1:E:224:VAL:O	1:E:228:VAL:HB	2.15	0.47
1:C:86:ALA:HA	1:C:105:PHE:HA	1.97	0.47
1:D:86:ALA:HA	1:D:105:PHE:HA	1.96	0.47
1:E:151:ASN:O	1:E:154:VAL:HG22	2.14	0.47
1:C:117:ARG:O	1:C:121:ASP:HB3	2.14	0.47
1:D:117:ARG:O	1:D:121:ASP:HB3	2.15	0.47
1:E:51:LEU:HD11	1:E:93:VAL:HG21	1.97	0.47
1:E:86:ALA:HA	1:E:105:PHE:HA	1.96	0.47
1:E:257:ILE:HG22	1:E:309:LEU:HD23	1.96	0.47
1:D:94:SER:N	1:D:98:THR:O	2.21	0.47
1:A:104:ARG:HD2	1:B:76:ARG:NH1	2.30	0.47
1:D:200:ILE:O	1:D:204:MET:HB2	2.15	0.47
1:E:200:ILE:O	1:E:204:MET:HB2	2.15	0.47
1:A:117:ARG:O	1:A:121:ASP:HB3	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:ASN:O	1:B:154:VAL:HG22	2.16	0.46
1:C:257:ILE:HG22	1:C:309:LEU:HD23	1.97	0.46
1:B:86:ALA:HA	1:B:105:PHE:HA	1.96	0.46
1:B:257:ILE:HG22	1:B:309:LEU:HD23	1.97	0.46
1:D:257:ILE:HG22	1:D:309:LEU:HD23	1.97	0.46
1:E:197:ILE:HB	1:E:198:PRO:HD3	1.97	0.46
1:A:18:ASN:HB3	1:A:143:VAL:HG23	1.98	0.46
1:B:23:LEU:N	1:B:149:GLY:O	2.48	0.46
1:C:18:ASN:HB3	1:C:143:VAL:HG23	1.97	0.46
1:A:257:ILE:HG22	1:A:309:LEU:HD23	1.98	0.46
1:B:197:ILE:HB	1:B:198:PRO:HD3	1.97	0.46
1:D:23:LEU:N	1:D:149:GLY:O	2.49	0.46
1:B:66:GLU:HG3	1:B:67:PRO:HD2	1.98	0.46
1:C:23:LEU:N	1:C:149:GLY:O	2.49	0.46
1:C:54:ASP:OD1	1:C:57:ARG:HB2	2.16	0.45
1:A:137:ARG:HA	1:A:137:ARG:HD3	1.82	0.45
1:C:66:GLU:HG3	1:C:67:PRO:HD2	1.98	0.45
1:E:23:LEU:N	1:E:149:GLY:O	2.48	0.45
1:A:151:ASN:O	1:A:154:VAL:HG22	2.16	0.45
1:D:224:VAL:O	1:D:228:VAL:HB	2.16	0.45
1:A:77:PHE:CD1	1:A:84:ARG:HD2	2.52	0.45
1:C:137:ARG:HA	1:C:137:ARG:HD3	1.82	0.45
1:D:21:ILE:HA	1:D:41:PHE:O	2.17	0.45
1:D:18:ASN:HB3	1:D:143:VAL:HG23	1.98	0.45
1:E:21:ILE:HA	1:E:41:PHE:O	2.17	0.45
1:E:66:GLU:HG3	1:E:67:PRO:HD2	1.97	0.45
1:D:66:GLU:HG3	1:D:67:PRO:HD2	1.98	0.45
1:D:141:LEU:HD23	1:D:142:ALA:H	1.81	0.45
1:A:23:LEU:N	1:A:149:GLY:O	2.50	0.45
1:A:197:ILE:HB	1:A:198:PRO:HD3	1.99	0.45
1:D:137:ARG:HA	1:D:137:ARG:HD3	1.82	0.45
1:D:197:ILE:HB	1:D:198:PRO:HD3	1.98	0.45
1:A:208:LEU:HD13	1:A:261:ILE:HG23	1.99	0.45
1:B:77:PHE:CD1	1:B:84:ARG:HD2	2.52	0.45
1:D:151:ASN:O	1:D:154:VAL:HG22	2.15	0.45
1:A:66:GLU:HG3	1:A:67:PRO:HD2	1.99	0.45
1:B:141:LEU:HD23	1:B:142:ALA:H	1.82	0.45
1:C:104:ARG:HD2	1:D:76:ARG:NH1	2.31	0.45
1:D:40:ALA:HB3	1:D:105:PHE:CZ	2.52	0.45
1:D:55:PRO:HG2	1:D:56:VAL:H	1.82	0.45
1:E:94:SER:HB3	1:E:98:THR:HB	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ASN:HB2	1:A:45:SER:OG	2.17	0.44
1:B:200:ILE:O	1:B:204:MET:HB2	2.16	0.44
1:B:21:ILE:HA	1:B:41:PHE:O	2.18	0.44
1:B:34:GLU:OE2	1:B:113:LEU:N	2.40	0.44
1:C:141:LEU:HD23	1:C:142:ALA:H	1.83	0.44
1:C:197:ILE:HB	1:C:198:PRO:HD3	1.99	0.44
1:B:208:LEU:HD13	1:B:261:ILE:HG23	1.99	0.44
1:C:21:ILE:HA	1:C:41:PHE:O	2.17	0.44
1:D:54:ASP:CG	1:D:57:ARG:HB2	2.43	0.44
1:C:245:LEU:HD12	1:C:245:LEU:HA	1.79	0.44
1:E:15:LEU:HD11	1:E:46:TRP:HB2	2.00	0.44
1:A:54:ASP:OD1	1:A:57:ARG:HB2	2.18	0.44
1:A:123:GLN:HB2	1:A:189:ILE:HG13	2.00	0.44
1:C:51:LEU:HD11	1:C:93:VAL:HG21	1.99	0.44
1:C:94:SER:HB3	1:C:98:THR:HB	1.99	0.44
1:C:208:LEU:HD13	1:C:261:ILE:HG23	1.99	0.44
1:B:18:ASN:HB3	1:B:143:VAL:HG23	1.99	0.43
1:E:54:ASP:OD1	1:E:57:ARG:HB2	2.18	0.43
1:A:104:ARG:HD2	1:B:76:ARG:HH11	1.83	0.43
1:B:51:LEU:HD11	1:B:93:VAL:HG21	2.00	0.43
1:C:119:PRO:HB2	1:C:120:PHE:CE1	2.53	0.43
1:C:149:GLY:HA3	1:C:164:PHE:CD2	2.54	0.43
1:B:27:TYR:HB3	1:C:110:LEU:HD11	2.00	0.43
1:B:309:LEU:HD12	1:B:309:LEU:HA	1.87	0.43
1:E:149:GLY:HA3	1:E:164:PHE:CD2	2.52	0.43
1:A:21:ILE:HA	1:A:41:PHE:O	2.18	0.43
1:D:48:ASP:N	1:D:97:GLY:O	2.37	0.43
1:A:40:ALA:HB3	1:A:105:PHE:CZ	2.53	0.43
1:A:44:LEU:HB2	1:A:101:TYR:HB3	2.01	0.43
1:B:267:VAL:HA	1:B:270:ILE:HB	2.01	0.43
1:A:34:GLU:OE2	1:A:113:LEU:N	2.42	0.43
1:B:149:GLY:HA3	1:B:164:PHE:CD2	2.53	0.43
1:D:149:GLY:HA3	1:D:164:PHE:CD2	2.54	0.43
1:E:40:ALA:HB3	1:E:105:PHE:CZ	2.53	0.43
1:E:208:LEU:HD13	1:E:261:ILE:HG23	2.01	0.43
1:B:304:LEU:O	1:B:308:ILE:HG12	2.19	0.42
1:E:129:LEU:O	1:E:182:LYS:HA	2.19	0.42
1:C:210:ILE:HG23	1:D:269:VAL:HG11	2.00	0.42
1:A:51:LEU:HD11	1:A:93:VAL:HG21	2.01	0.42
1:A:245:LEU:HD12	1:A:245:LEU:HA	1.82	0.42
1:C:123:GLN:HB2	1:C:189:ILE:HG13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:115:PHE:O	1:E:252:THR:HG22	2.19	0.42
1:A:141:LEU:HD23	1:A:142:ALA:H	1.84	0.42
1:A:119:PRO:HB2	1:A:120:PHE:CE1	2.54	0.42
1:B:94:SER:HB3	1:B:98:THR:HB	2.00	0.42
1:C:15:LEU:HD11	1:C:46:TRP:HB2	2.02	0.42
1:C:104:ARG:HD2	1:D:76:ARG:HH11	1.85	0.42
1:D:52:ALA:HB1	1:D:95:PRO:O	2.20	0.42
1:D:77:PHE:CD1	1:D:84:ARG:HD2	2.54	0.42
1:E:137:ARG:HA	1:E:137:ARG:HD3	1.82	0.42
1:B:119:PRO:HB2	1:B:120:PHE:CE1	2.54	0.42
1:D:15:LEU:HD11	1:D:46:TRP:HB2	2.01	0.42
1:D:245:LEU:HD12	1:D:245:LEU:HA	1.79	0.42
1:E:18:ASN:HB3	1:E:143:VAL:HG23	2.01	0.42
1:B:54:ASP:OD1	1:B:57:ARG:HB2	2.19	0.42
1:A:256:ALA:HB1	1:A:309:LEU:HD21	2.01	0.42
1:C:151:ASN:C	1:C:153:ASP:H	2.28	0.42
1:E:18:ASN:HB2	1:E:45:SER:OG	2.20	0.42
1:B:40:ALA:HB3	1:B:105:PHE:CZ	2.55	0.42
1:D:129:LEU:O	1:D:182:LYS:HA	2.20	0.42
1:C:77:PHE:CD1	1:C:84:ARG:HD2	2.55	0.41
1:D:123:GLN:HB2	1:D:189:ILE:HG13	2.01	0.41
1:E:77:PHE:CD1	1:E:84:ARG:HD2	2.54	0.41
1:A:309:LEU:HD12	1:A:309:LEU:HA	1.88	0.41
1:C:40:ALA:HB3	1:C:105:PHE:CZ	2.55	0.41
1:D:18:ASN:HB2	1:D:45:SER:OG	2.20	0.41
1:D:119:PRO:HB2	1:D:120:PHE:CE1	2.55	0.41
1:B:151:ASN:C	1:B:153:ASP:H	2.29	0.41
1:D:115:PHE:O	1:D:252:THR:HG22	2.20	0.41
1:E:151:ASN:C	1:E:153:ASP:H	2.28	0.41
1:A:25:GLU:HB2	1:A:39:ASN:HB3	2.03	0.41
1:B:15:LEU:HD11	1:B:46:TRP:HB2	2.02	0.41
1:B:129:LEU:O	1:B:182:LYS:HA	2.21	0.41
1:D:151:ASN:C	1:D:153:ASP:H	2.29	0.41
1:C:149:GLY:HA3	1:C:164:PHE:HD2	1.85	0.41
1:A:15:LEU:HD11	1:A:46:TRP:HB2	2.02	0.41
1:B:18:ASN:HB2	1:B:45:SER:OG	2.21	0.41
1:C:115:PHE:O	1:C:252:THR:HG22	2.21	0.41
1:A:149:GLY:HA3	1:A:164:PHE:CD2	2.56	0.41
1:B:123:GLN:HB2	1:B:189:ILE:HG13	2.02	0.41
1:C:18:ASN:HB2	1:C:45:SER:OG	2.20	0.41
1:C:267:VAL:HA	1:C:270:ILE:HB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:65:TYR:CG	1:E:70:ILE:HD11	2.56	0.41
1:E:149:GLY:HA3	1:E:164:PHE:HD2	1.85	0.41
1:B:137:ARG:HD3	1:B:137:ARG:HA	1.81	0.41
1:C:27:TYR:HB3	1:D:110:LEU:HD11	2.03	0.41
1:C:119:PRO:HB2	1:C:120:PHE:CD1	2.56	0.41
1:C:129:LEU:O	1:C:182:LYS:HA	2.20	0.41
1:D:149:GLY:HA3	1:D:164:PHE:HD2	1.86	0.41
1:C:65:TYR:CG	1:C:70:ILE:HD11	2.56	0.40
1:D:309:LEU:HD12	1:D:309:LEU:HA	1.89	0.40
1:E:119:PRO:HB2	1:E:120:PHE:CE1	2.55	0.40
1:B:115:PHE:O	1:B:252:THR:HG22	2.22	0.40
1:B:149:GLY:HA3	1:B:164:PHE:HD2	1.86	0.40
1:A:84:ARG:H	1:A:84:ARG:HG2	1.66	0.40
1:A:151:ASN:C	1:A:153:ASP:H	2.29	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	308/316 (98%)	283 (92%)	24 (8%)	1 (0%)	36	65
1	B	308/316 (98%)	283 (92%)	24 (8%)	1 (0%)	36	65
1	C	308/316 (98%)	283 (92%)	24 (8%)	1 (0%)	36	65
1	D	308/316 (98%)	283 (92%)	24 (8%)	1 (0%)	36	65
1	E	308/316 (98%)	283 (92%)	24 (8%)	1 (0%)	36	65
All	All	1540/1580 (98%)	1415 (92%)	120 (8%)	5 (0%)	36	65

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%)	256 (92%)	21 (8%)	12	37
1	B	277/283 (98%)	256 (92%)	21 (8%)	12	37
1	C	277/283 (98%)	256 (92%)	21 (8%)	12	37
1	D	277/283 (98%)	257 (93%)	20 (7%)	13	40
1	E	277/283 (98%)	256 (92%)	21 (8%)	12	37
All	All	1385/1415 (98%)	1281 (92%)	104 (8%)	12	38

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	ASP
1	A	64	THR
1	A	68	GLU
1	A	84	ARG
1	A	110	LEU
1	A	120	PHE
1	A	124	THR
1	A	134	VAL
1	A	141	LEU
1	A	150	LYS
1	A	157	THR
1	A	177	ASP
1	A	193	TYR
1	A	202	LEU
1	A	211	SER

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Mol	Chain	Res	Type
1	A	213	THR
1	A	221	GLU
1	A	226	LEU
1	A	254	THR
1	A	274	VAL
1	A	292	ARG
1	B	54	ASP
1	B	64	THR
1	B	68	GLU
1	B	84	ARG
1	B	110	LEU
1	B	120	PHE
1	B	124	THR
1	B	134	VAL
1	B	141	LEU
1	B	150	LYS
1	B	157	THR
1	B	177	ASP
1	B	193	TYR
1	B	202	LEU
1	B	211	SER
1	B	213	THR
1	B	221	GLU
1	B	226	LEU
1	B	254	THR
1	B	274	VAL
1	B	292	ARG
1	C	54	ASP
1	C	64	THR
1	C	68	GLU
1	C	84	ARG
1	C	110	LEU
1	C	120	PHE
1	C	124	THR
1	C	134	VAL
1	C	141	LEU
1	C	150	LYS
1	C	157	THR
1	C	177	ASP
1	C	193	TYR
1	C	202	LEU
1	C	211	SER

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Mol	Chain	Res	Type
1	C	213	THR
1	C	221	GLU
1	C	226	LEU
1	C	254	THR
1	C	274	VAL
1	C	292	ARG
1	D	64	THR
1	D	68	GLU
1	D	84	ARG
1	D	110	LEU
1	D	120	PHE
1	D	124	THR
1	D	134	VAL
1	D	141	LEU
1	D	150	LYS
1	D	157	THR
1	D	177	ASP
1	D	193	TYR
1	D	202	LEU
1	D	211	SER
1	D	213	THR
1	D	221	GLU
1	D	226	LEU
1	D	254	THR
1	D	274	VAL
1	D	292	ARG
1	E	54	ASP
1	E	64	THR
1	E	68	GLU
1	E	84	ARG
1	E	110	LEU
1	E	120	PHE
1	E	124	THR
1	E	134	VAL
1	E	141	LEU
1	E	150	LYS
1	E	157	THR
1	E	177	ASP
1	E	193	TYR
1	E	202	LEU
1	E	211	SER
1	E	213	THR

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Mol	Chain	Res	Type
1	E	221	GLU
1	E	226	LEU
1	E	254	THR
1	E	274	VAL
1	E	292	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	GLN
1	A	234	HIS
1	B	123	GLN
1	C	123	GLN
1	C	306	ASN
1	D	123	GLN
1	E	123	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	0.98	53 (17%) 4 4	59, 92, 140, 181	0
1	B	310/316 (98%)	0.93	39 (12%) 8 6	56, 91, 141, 177	0
1	C	310/316 (98%)	1.06	55 (17%) 4 3	62, 91, 155, 209	0
1	D	310/316 (98%)	1.28	69 (22%) 2 2	59, 90, 132, 179	0
1	E	310/316 (98%)	0.89	36 (11%) 9 8	58, 91, 138, 182	0
All	All	1550/1580 (98%)	1.03	252 (16%) 4 4	56, 91, 142, 209	0

All (252) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	148	VAL	8.4
1	C	60	VAL	7.0
1	D	148	VAL	6.3
1	A	141	LEU	6.1
1	D	45	SER	6.0
1	C	155	PHE	5.9
1	C	59	GLY	5.9
1	A	148	VAL	5.7
1	E	148	VAL	5.5
1	A	7	PRO	5.4
1	B	153	ASP	5.4
1	D	18	ASN	5.1
1	E	59	GLY	5.1
1	D	11	ALA	5.1
1	C	74	GLU	5.1
1	A	134	VAL	5.0
1	A	173	PHE	4.9
1	C	138	ASN	4.8
1	D	211	SER	4.8
1	D	208	LEU	4.8

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Mol	Chain	Res	Type	RSRZ
1	C	148	VAL	4.7
1	E	144	ASP	4.7
1	D	207	ILE	4.7
1	C	7	PRO	4.7
1	D	7	PRO	4.7
1	B	11	ALA	4.6
1	E	155	PHE	4.5
1	A	211	SER	4.4
1	D	315	GLY	4.4
1	E	134	VAL	4.3
1	D	206	PHE	4.3
1	A	155	PHE	4.3
1	D	155	PHE	4.2
1	B	152	ASP	4.2
1	D	230	THR	4.2
1	D	144	ASP	4.1
1	A	74	GLU	4.1
1	E	87	ASP	4.1
1	B	144	ASP	4.0
1	D	55	PRO	4.0
1	A	145	LEU	3.9
1	A	208	LEU	3.9
1	C	285	ALA	3.9
1	E	7	PRO	3.8
1	B	18	ASN	3.8
1	D	47	LYS	3.8
1	E	147	LYS	3.8
1	E	136	THR	3.8
1	E	173	PHE	3.7
1	B	155	PHE	3.7
1	B	315	GLY	3.7
1	D	60	VAL	3.7
1	C	141	LEU	3.7
1	D	94	SER	3.6
1	D	146	GLU	3.6
1	D	186	GLN	3.6
1	A	281	GLU	3.6
1	B	211	SER	3.6
1	E	60	VAL	3.6
1	D	101	TYR	3.6
1	E	138	ASN	3.5
1	A	219	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	47	LYS	3.5
1	A	230	THR	3.5
1	D	51	LEU	3.5
1	C	173	PHE	3.5
1	E	47	LYS	3.5
1	C	214	ALA	3.5
1	E	214	ALA	3.5
1	A	212	TRP	3.5
1	A	87	ASP	3.4
1	B	54	ASP	3.4
1	C	131	VAL	3.4
1	A	64	THR	3.4
1	B	141	LEU	3.4
1	D	33	ALA	3.4
1	A	316	PHE	3.4
1	A	144	ASP	3.3
1	B	277	TYR	3.3
1	D	19	THR	3.2
1	A	13	GLU	3.2
1	D	209	PHE	3.2
1	D	100	GLN	3.2
1	C	279	LYS	3.2
1	D	95	PRO	3.2
1	E	221	GLU	3.1
1	A	206	PHE	3.1
1	D	108	ARG	3.1
1	A	209	PHE	3.1
1	B	12	ASP	3.1
1	B	57	ARG	3.1
1	B	142	ALA	3.0
1	D	44	LEU	3.0
1	C	11	ALA	3.0
1	A	223	ASN	3.0
1	A	88	VAL	3.0
1	D	53	PHE	3.0
1	D	25	GLU	3.0
1	D	212	TRP	3.0
1	C	280	VAL	3.0
1	A	133	SER	3.0
1	B	177	ASP	3.0
1	A	60	VAL	3.0
1	E	186	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	173	PHE	3.0
1	C	63	LYS	2.9
1	B	316	PHE	2.9
1	D	12	ASP	2.9
1	B	7	PRO	2.9
1	C	211	SER	2.9
1	E	145	LEU	2.9
1	C	90	ASP	2.9
1	D	30	ASP	2.9
1	A	176	GLU	2.9
1	A	152	ASP	2.9
1	A	177	ASP	2.9
1	C	13	GLU	2.9
1	C	73	PRO	2.8
1	B	242	GLU	2.8
1	C	130	ILE	2.8
1	D	153	ASP	2.8
1	E	266	PHE	2.8
1	A	11	ALA	2.8
1	B	140	VAL	2.8
1	D	141	LEU	2.8
1	D	246	ALA	2.8
1	A	143	VAL	2.8
1	D	281	GLU	2.8
1	D	59	GLY	2.7
1	A	207	ILE	2.7
1	C	61	ARG	2.7
1	E	139	ILE	2.7
1	D	136	THR	2.7
1	D	242	GLU	2.7
1	C	291	THR	2.7
1	C	82	ASN	2.7
1	C	181	SER	2.7
1	B	74	GLU	2.6
1	E	212	TRP	2.6
1	D	145	LEU	2.6
1	A	138	ASN	2.6
1	A	25	GLU	2.6
1	C	10	ILE	2.6
1	B	173	PHE	2.6
1	D	135	ASP	2.6
1	A	65	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	138	ASN	2.6
1	E	141	LEU	2.6
1	B	221	GLU	2.6
1	D	88	VAL	2.6
1	E	56	VAL	2.6
1	D	194	PHE	2.5
1	D	210	ILE	2.5
1	D	26	CYS	2.5
1	D	56	VAL	2.5
1	B	244	ASN	2.5
1	D	142	ALA	2.5
1	E	74	GLU	2.5
1	E	316	PHE	2.5
1	C	83	ALA	2.5
1	D	57	ARG	2.5
1	D	112	PRO	2.5
1	A	142	ALA	2.4
1	D	187	LEU	2.4
1	C	284	PRO	2.4
1	C	316	PHE	2.4
1	C	18	ASN	2.4
1	C	277	TYR	2.4
1	E	65	TYR	2.4
1	C	288	ALA	2.4
1	A	63	LYS	2.4
1	A	221	GLU	2.4
1	E	176	GLU	2.4
1	D	126	HIS	2.4
1	D	84	ARG	2.4
1	B	81	GLU	2.4
1	B	138	ASN	2.4
1	A	222	ALA	2.4
1	D	316	PHE	2.4
1	A	62	VAL	2.4
1	A	218	THR	2.3
1	C	54	ASP	2.3
1	D	48	ASP	2.3
1	A	214	ALA	2.3
1	B	10	ILE	2.3
1	D	52	ALA	2.3
1	E	11	ALA	2.3
1	C	193	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	153	ASP	2.3
1	B	137	ARG	2.3
1	C	28	SER	2.3
1	D	10	ILE	2.3
1	D	63	LYS	2.3
1	C	296	ILE	2.3
1	C	26	CYS	2.3
1	A	135	ASP	2.3
1	C	153	ASP	2.3
1	C	275	GLN	2.3
1	A	147	LYS	2.3
1	C	25	GLU	2.3
1	D	81	GLU	2.3
1	E	58	SER	2.3
1	A	140	VAL	2.3
1	C	56	VAL	2.3
1	C	87	ASP	2.3
1	C	144	ASP	2.3
1	D	140	VAL	2.3
1	A	315	GLY	2.2
1	E	84	ARG	2.2
1	C	221	GLU	2.2
1	D	130	ILE	2.2
1	C	101	TYR	2.2
1	D	282	SER	2.2
1	D	65	TYR	2.2
1	C	282	SER	2.2
1	E	13	GLU	2.2
1	A	12	ASP	2.2
1	B	194	PHE	2.2
1	C	206	PHE	2.2
1	C	140	VAL	2.2
1	E	242	GLU	2.2
1	B	193	TYR	2.1
1	A	139	ILE	2.1
1	D	73	PRO	2.1
1	B	53	PHE	2.1
1	B	145	LEU	2.1
1	C	208	LEU	2.1
1	D	304	LEU	2.1
1	A	174	ALA	2.1
1	B	59	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	225	THR	2.1
1	B	136	THR	2.1
1	C	27	TYR	2.1
1	C	51	LEU	2.1
1	E	263	LEU	2.1
1	B	275	GLN	2.1
1	C	209	PHE	2.1
1	B	224	VAL	2.1
1	A	277	TYR	2.1
1	E	165	THR	2.1
1	D	13	GLU	2.1
1	B	87	ASP	2.1
1	A	265	TYR	2.1
1	A	19	THR	2.0
1	C	85	ASP	2.0
1	C	273	THR	2.0
1	D	124	THR	2.0
1	E	315	GLY	2.0
1	C	32	LYS	2.0
1	E	217	SER	2.0
1	B	212	TRP	2.0
1	E	247	LYS	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.