



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 17, 2025 – 02:15 PM EDT

PDB ID : 9NS6 / pdb\_00009ns6  
Title : KslB apoenzyme  
Authors : Kim, K.; Kim, W.  
Deposited on : 2025-03-16  
Resolution : 2.95 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

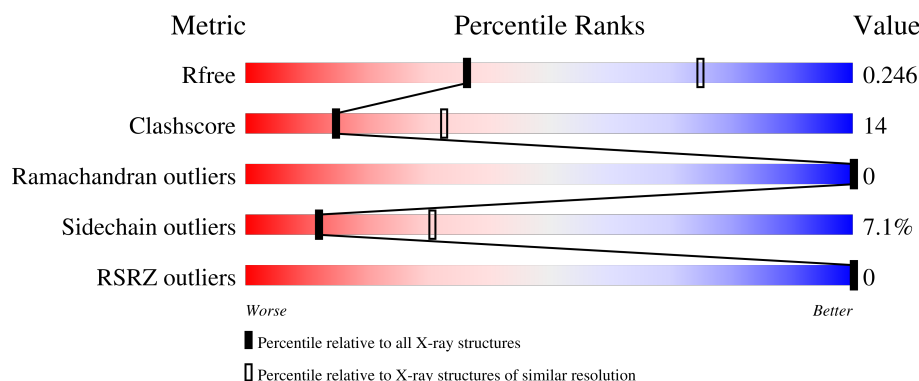
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.95 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))
$R_{free}$	164625	1044 (2.98-2.94)
Clashscore	180529	1097 (2.98-2.94)
Ramachandran outliers	177936	1049 (2.98-2.94)
Sidechain outliers	177891	1049 (2.98-2.94)
RSRZ outliers	164620	1044 (2.98-2.94)

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  $\geq 3$ , 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	317	
1	B	317	
1	C	317	
1	D	317	
1	E	317	

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Mol	Chain	Length	Quality of chain
1	F	317	 A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: green (49%), yellow (35%), and orange (12%). The segments are labeled with their respective percentages: 49%, 35%, and 12%.

## 2 Entry composition

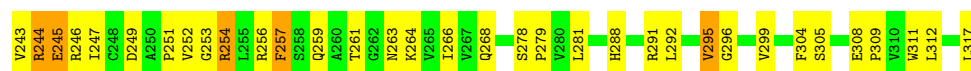
There is only 1 type of molecule in this entry. The entry contains 13615 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Pictet-Spenglerase.

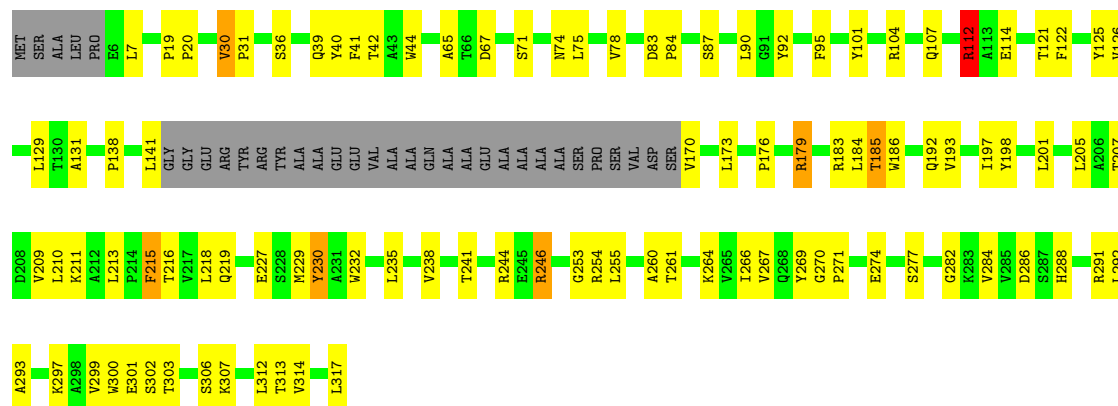
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	293	Total	C	N	O	S	0	0	0
			2307	1478	388	437	4			
1	B	287	Total	C	N	O	S	0	0	0
			2262	1447	382	429	4			
1	C	292	Total	C	N	O	S	0	0	0
			2318	1484	391	440	3			
1	D	284	Total	C	N	O	S	0	0	0
			2252	1443	379	427	3			
1	E	286	Total	C	N	O	S	0	0	0
			2259	1449	378	429	3			
1	F	279	Total	C	N	O	S	0	0	0
			2217	1422	371	421	3			





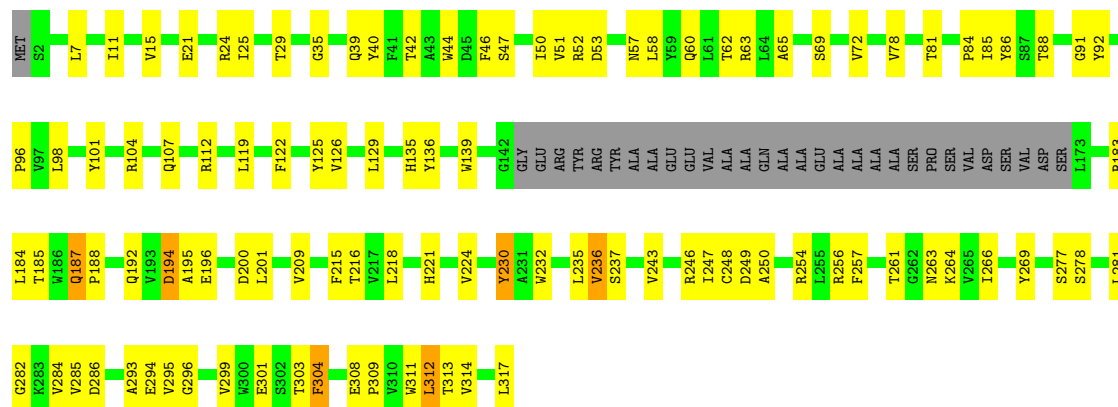
- Molecule 1: Pictet-Spenglerase

Chain D:  58% 29% • 10%



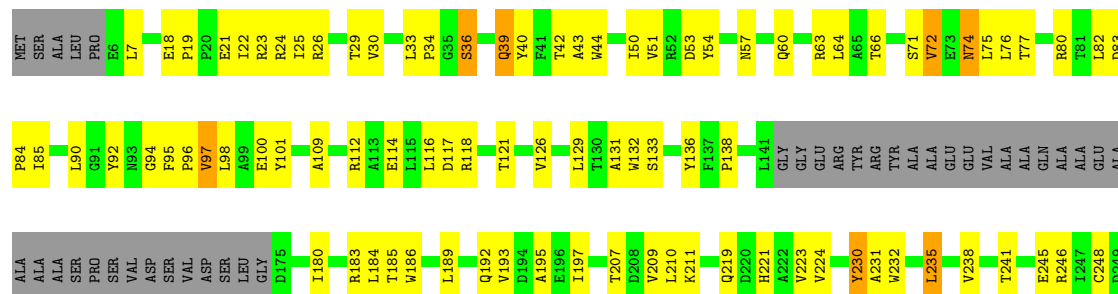
- Molecule 1: Pictet-Spenglerase

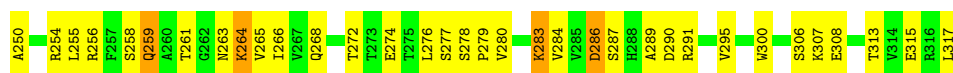
Chain E:  57% 32% 10%



- Molecule 1: Pictet-Spenglerase

Chain F:  49% 35% • 12%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.59Å 95.59Å 193.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.80 – 2.95 47.80 – 2.95	Depositor EDS
% Data completeness (in resolution range)	96.2 (47.80-2.95) 96.2 (47.80-2.95)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.43 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, $R_{free}$	0.207 , 0.248 0.205 , 0.246	Depositor DCC
$R_{free}$ test set	38045 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.0	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 31.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.067 for -h,-k,l 0.448 for h,-h-k,-l 0.068 for -k,-h,-l	Xtriage
Reported twinning fraction	0.490 for h,-h-k,-l	Depositor
Outliers	0 of 40059 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13615	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 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	0.61	0/2367	0.60	0/3241
1	B	0.61	0/2319	0.61	0/3174
1	C	0.61	0/2379	0.62	0/3254
1	D	0.61	0/2311	0.62	0/3164
1	E	0.61	0/2319	0.65	0/3176
1	F	0.63	0/2276	0.66	0/3117
All	All	0.61	0/13971	0.63	0/19126

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	2
1	C	0	3
1	D	0	1
All	All	0	9

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	118	ARG	Sidechain
1	A	52	ARG	Sidechain
1	A	80	ARG	Sidechain
1	B	179	ARG	Sidechain
1	B	63	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	C	244	ARG	Sidechain
1	C	246	ARG	Sidechain
1	C	80	ARG	Sidechain
1	D	112	ARG	Sidechain

## 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	2307	0	2264	45	0
1	B	2262	0	2226	50	0
1	C	2318	0	2263	57	0
1	D	2252	0	2208	68	0
1	E	2259	0	2214	75	0
1	F	2217	0	2169	96	0
All	All	13615	0	13344	366	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 14.

All (366) 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:F:184:LEU:HB2	1:F:193:VAL:HG22	1.45	0.99
1:F:63:ARG:HG2	1:F:238:VAL:HG23	1.47	0.96
1:E:62:THR:HG22	1:E:119:LEU:HB3	1.55	0.87
1:E:221:HIS:H	1:E:303:THR:HG21	1.49	0.77
1:F:246:ARG:HA	1:F:277:SER:HA	1.67	0.76
1:F:185:THR:HG22	1:F:192:GLN:HG2	1.68	0.75
1:B:65:ALA:HB3	1:B:116:LEU:HD13	1.68	0.75
1:C:176:PRO:HA	1:C:179:ARG:HE	1.52	0.75
1:E:209:VAL:HG11	1:E:281:LEU:HD11	1.70	0.73
1:E:256:ARG:HD2	1:E:278:SER:HB3	1.71	0.72
1:A:230:TYR:HB3	1:A:266:ILE:HG12	1.71	0.72
1:B:179:ARG:HG2	1:B:198:TYR:HA	1.72	0.71
1:D:284:VAL:HG21	1:D:292:LEU:HD22	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:LEU:HB3	1:B:191:VAL:HG23	1.74	0.69
1:F:223:VAL:HG23	1:F:224:VAL:HG23	1.77	0.67
1:A:256:ARG:HD2	1:A:278:SER:HB3	1.76	0.67
1:A:61:LEU:HD13	1:A:79:PHE:HD1	1.60	0.66
1:E:183:ARG:HB2	1:E:317:LEU:HD11	1.78	0.66
1:C:185:THR:HG23	1:C:192:GLN:HG2	1.76	0.66
1:F:25:ILE:HD11	1:F:94:GLY:HA3	1.78	0.66
1:D:30:VAL:HG12	1:D:31:PRO:HD2	1.78	0.65
1:D:71:SER:O	1:D:75:LEU:HD13	1.97	0.65
1:F:221:HIS:CE1	1:F:300:TRP:HD1	2.14	0.65
1:E:246:ARG:HB3	1:E:249:ASP:HB2	1.80	0.64
1:C:145:ARG:HD2	1:D:141:LEU:HD21	1.80	0.64
1:D:176:PRO:HA	1:D:179:ARG:CD	2.27	0.64
1:E:88:THR:OG1	1:F:276:LEU:HD21	1.98	0.63
1:D:210:LEU:HD23	1:D:213:LEU:HD12	1.81	0.63
1:B:269:TYR:CZ	1:B:296:GLY:HA3	2.32	0.63
1:D:65:ALA:HA	1:D:75:LEU:HD21	1.80	0.62
1:E:221:HIS:HB2	1:E:299:VAL:HG12	1.81	0.62
1:E:301:GLU:HA	1:E:304:PHE:HB2	1.81	0.62
1:F:19:PRO:HD2	1:F:22:ILE:HD11	1.83	0.60
1:F:66:THR:HG21	1:F:238:VAL:HG21	1.82	0.60
1:D:299:VAL:HA	1:D:302:SER:HB3	1.84	0.60
1:B:126:VAL:HA	1:B:129:LEU:HD12	1.82	0.60
1:D:101:TYR:HA	1:D:104:ARG:HD2	1.83	0.60
1:B:26:ARG:HD3	1:B:136:TYR:HB3	1.82	0.59
1:C:223:VAL:HG23	1:C:224:VAL:HG13	1.82	0.59
1:E:91:GLY:HA2	1:E:96:PRO:HA	1.84	0.59
1:B:72:VAL:HG13	1:B:115:LEU:HD12	1.84	0.59
1:C:256:ARG:HB2	1:C:266:ILE:HG23	1.84	0.59
1:F:207:THR:O	1:F:211:LYS:HG3	2.03	0.59
1:A:178:GLN:HE21	1:A:178:GLN:HA	1.67	0.59
1:E:269:TYR:CZ	1:E:296:GLY:HA3	2.38	0.59
1:F:85:ILE:HD12	1:F:85:ILE:H	1.68	0.58
1:F:23:ARG:HD3	1:F:26:ARG:HH21	1.69	0.58
1:F:219:GLN:OE1	1:F:231:ALA:HB2	2.04	0.58
1:F:250:ALA:HB3	1:F:268:GLN:HE22	1.68	0.58
1:A:261:THR:O	1:A:264:LYS:HE2	2.04	0.58
1:E:57:ASN:ND2	1:F:57:ASN:HD21	2.02	0.58
1:C:8:ARG:HA	1:C:11:ILE:HD12	1.85	0.57
1:C:186:TRP:HZ3	1:C:193:VAL:HG13	1.68	0.57
1:E:46:PHE:O	1:E:50:ILE:HB	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:269:TYR:HD2	1:E:293:ALA:HA	1.69	0.57
1:F:34:PRO:HB2	1:F:43:ALA:HB1	1.86	0.57
1:E:84:PRO:O	1:E:88:THR:HG22	2.04	0.57
1:F:72:VAL:HG21	1:F:112:ARG:HA	1.85	0.57
1:E:126:VAL:HA	1:E:129:LEU:HD12	1.86	0.57
1:F:256:ARG:NH2	1:F:268:GLN:HE21	2.02	0.57
1:D:185:THR:HB	1:D:192:GLN:HG3	1.85	0.57
1:F:186:TRP:HZ3	1:F:193:VAL:HG13	1.70	0.57
1:E:57:ASN:HD21	1:F:57:ASN:HD21	1.52	0.57
1:C:184:LEU:HB2	1:C:193:VAL:HG22	1.86	0.56
1:F:183:ARG:HB2	1:F:317:LEU:HD11	1.86	0.56
1:B:194:ASP:O	1:B:285:VAL:HG22	2.06	0.56
1:D:122:PHE:O	1:D:126:VAL:HG23	2.05	0.56
1:E:86:TYR:OH	1:F:53:ASP:HB3	2.04	0.56
1:B:195:ALA:HA	1:B:284:VAL:HA	1.88	0.56
1:A:184:LEU:HB2	1:A:193:VAL:HG22	1.88	0.55
1:D:267:VAL:HG11	1:D:292:LEU:HD11	1.89	0.55
1:D:269:TYR:HB2	1:D:293:ALA:HA	1.87	0.55
1:D:230:TYR:HB3	1:D:266:ILE:HG12	1.89	0.55
1:F:22:ILE:CD1	1:F:132:TRP:HB3	2.37	0.54
1:F:184:LEU:HB2	1:F:193:VAL:CG2	2.29	0.54
1:B:54:TYR:HE2	1:B:98:LEU:HD21	1.73	0.54
1:F:26:ARG:HG3	1:F:44:TRP:CH2	2.42	0.54
1:C:219:GLN:HE22	1:C:312:LEU:HD22	1.72	0.54
1:E:232:TRP:CE2	1:E:264:LYS:HD3	2.43	0.54
1:B:54:TYR:CE2	1:B:98:LEU:HD21	2.43	0.54
1:E:11:ILE:O	1:E:15:VAL:HG23	2.08	0.54
1:E:78:VAL:HA	1:F:64:LEU:HD11	1.90	0.54
1:A:194:ASP:O	1:A:285:VAL:HG13	2.08	0.54
1:C:143:GLY:HA3	1:C:304:PHE:HZ	1.73	0.54
1:E:21:GLU:O	1:E:25:ILE:HG13	2.08	0.54
1:E:60:GLN:HA	1:E:63:ARG:HG2	1.89	0.54
1:E:235:LEU:HD12	1:E:237:SER:H	1.73	0.54
1:E:185:THR:HG23	1:E:192:GLN:HB3	1.90	0.53
1:C:50:ILE:HG23	1:C:86:TYR:HD2	1.73	0.53
1:E:295:VAL:O	1:E:299:VAL:HG23	2.07	0.53
1:D:7:LEU:HD11	1:D:125:TYR:CG	2.43	0.53
1:B:184:LEU:HG	1:B:314:VAL:HG22	1.91	0.53
1:B:209:VAL:HG11	1:B:281:LEU:HD21	1.91	0.53
1:C:139:TRP:CE3	1:D:42:THR:HG22	2.43	0.53
1:D:183:ARG:HB2	1:D:317:LEU:HD21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:74:ASN:O	1:D:78:VAL:HG23	2.08	0.53
1:F:26:ARG:HD3	1:F:136:TYR:HB3	1.91	0.53
1:C:145:ARG:HG2	1:E:69:SER:HA	1.91	0.53
1:D:246:ARG:HA	1:D:277:SER:HA	1.91	0.53
1:D:198:TYR:HD2	1:D:201:LEU:HD12	1.74	0.53
1:D:205:LEU:O	1:D:209:VAL:HG23	2.09	0.52
1:F:63:ARG:HG2	1:F:238:VAL:CG2	2.31	0.52
1:F:126:VAL:HA	1:F:129:LEU:HD12	1.92	0.52
1:B:114:GLU:O	1:B:118:ARG:HG3	2.10	0.52
1:D:7:LEU:HD23	1:D:121:THR:HG22	1.92	0.52
1:E:215:PHE:O	1:E:313:THR:HA	2.10	0.52
1:E:104:ARG:O	1:E:107:GLN:HG2	2.10	0.52
1:B:223:VAL:HG23	1:B:224:VAL:HG23	1.92	0.52
1:E:7:LEU:HD22	1:E:125:TYR:CD1	2.45	0.52
1:F:230:TYR:HB3	1:F:266:ILE:HG12	1.92	0.52
1:F:306:SER:HB3	1:F:308:GLU:HG2	1.92	0.52
1:F:22:ILE:HD13	1:F:132:TRP:HB3	1.92	0.51
1:F:248:CYS:HA	1:F:272:THR:HG23	1.93	0.51
1:F:255:LEU:HD11	1:F:284:VAL:HG23	1.91	0.51
1:F:40:TYR:O	1:F:44:TRP:N	2.36	0.51
1:C:147:ARG:HA	1:D:39:GLN:HA	1.92	0.51
1:A:65:ALA:HB3	1:A:116:LEU:HD13	1.92	0.51
1:F:18:GLU:HG3	1:F:22:ILE:HD11	1.93	0.51
1:B:176:PRO:HA	1:B:179:ARG:HD3	1.93	0.51
1:E:246:ARG:HA	1:E:277:SER:HA	1.92	0.51
1:E:269:TYR:CD2	1:E:293:ALA:HA	2.46	0.51
1:E:230:TYR:HB3	1:E:266:ILE:HG13	1.93	0.51
1:C:44:TRP:HZ2	1:C:136:TYR:O	1.94	0.50
1:C:230:TYR:CG	1:C:264:LYS:HE3	2.45	0.50
1:B:189:LEU:HD13	1:B:295:VAL:HG13	1.93	0.50
1:E:47:SER:O	1:E:51:VAL:HG12	2.12	0.50
1:D:104:ARG:HA	1:D:107:GLN:HG2	1.94	0.50
1:A:122:PHE:O	1:A:126:VAL:HG23	2.12	0.50
1:A:49:SER:HB3	1:B:49:SER:HB2	1.92	0.50
1:C:54:TYR:CD1	1:C:86:TYR:HB2	2.47	0.50
1:E:58:LEU:O	1:E:62:THR:HG23	2.11	0.50
1:F:44:TRP:CZ2	1:F:138:PRO:HD3	2.46	0.50
1:A:223:VAL:HG23	1:A:224:VAL:HG23	1.94	0.50
1:A:246:ARG:HH21	1:A:275:THR:HB	1.76	0.50
1:F:44:TRP:CH2	1:F:138:PRO:HD3	2.47	0.50
1:B:230:TYR:CG	1:B:264:LYS:HD2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:36:SER:O	1:D:39:GLN:HG3	2.11	0.49
1:D:176:PRO:HA	1:D:179:ARG:HD3	1.94	0.49
1:A:186:TRP:CD2	1:A:295:VAL:HG11	2.47	0.49
1:C:181:PRO:HG2	1:C:317:LEU:O	2.12	0.49
1:D:126:VAL:HA	1:D:129:LEU:HD12	1.93	0.49
1:F:256:ARG:HD2	1:F:278:SER:HB3	1.94	0.49
1:C:245:GLU:N	1:C:278:SER:O	2.45	0.49
1:E:21:GLU:O	1:E:24:ARG:HG2	2.13	0.49
1:E:196:GLU:O	1:E:282:GLY:HA3	2.13	0.49
1:E:135:HIS:CG	1:E:218:LEU:HD21	2.47	0.49
1:C:148:TYR:CE2	1:D:40:TYR:HB3	2.48	0.49
1:C:288:HIS:CE1	1:C:291:ARG:NH2	2.81	0.49
1:D:215:PHE:HD1	1:D:216:THR:H	1.60	0.49
1:F:54:TYR:HE2	1:F:98:LEU:HD21	1.77	0.49
1:C:186:TRP:CZ3	1:C:193:VAL:HG13	2.48	0.49
1:D:207:THR:O	1:D:211:LYS:HG3	2.13	0.49
1:F:97:VAL:HA	1:F:100:GLU:HG2	1.95	0.49
1:F:195:ALA:HB2	1:F:284:VAL:HG22	1.94	0.49
1:B:205:LEU:HD11	1:B:257:PHE:HD2	1.78	0.49
1:C:244:ARG:HA	1:C:279:PRO:HA	1.94	0.49
1:E:184:LEU:HG	1:E:314:VAL:HG22	1.95	0.49
1:F:250:ALA:HB3	1:F:268:GLN:NE2	2.28	0.48
1:C:140:ASP:HA	1:C:304:PHE:CZ	2.48	0.48
1:C:142:GLY:HA3	1:D:41:PHE:CB	2.43	0.48
1:C:229:MET:SD	1:C:296:GLY:HA2	2.53	0.48
1:F:195:ALA:HA	1:F:284:VAL:HA	1.96	0.48
1:F:254:ARG:HA	1:F:283:LYS:HG2	1.96	0.48
1:D:297:LYS:HZ3	1:D:300:TRP:HE3	1.60	0.48
1:B:21:GLU:O	1:B:25:ILE:HG13	2.14	0.48
1:E:60:GLN:OE1	1:E:63:ARG:HD3	2.13	0.48
1:E:88:THR:HG23	1:F:276:LEU:HD11	1.95	0.48
1:F:97:VAL:HA	1:F:100:GLU:CG	2.44	0.48
1:C:176:PRO:HA	1:C:179:ARG:NE	2.25	0.48
1:D:267:VAL:CG1	1:D:292:LEU:HD21	2.43	0.48
1:E:7:LEU:O	1:E:11:ILE:HG13	2.13	0.48
1:A:76:LEU:HB3	1:A:80:ARG:CZ	2.43	0.48
1:B:7:LEU:O	1:B:11:ILE:HG13	2.13	0.48
1:D:193:VAL:HB	1:D:288:HIS:HB3	1.96	0.48
1:D:216:THR:HG22	1:D:313:THR:HG23	1.96	0.48
1:C:122:PHE:O	1:C:126:VAL:HG23	2.14	0.47
1:F:209:VAL:HG22	1:F:235:LEU:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:245:GLU:OE2	1:F:250:ALA:HB2	2.14	0.47
1:F:131:ALA:HB2	1:F:232:TRP:CD2	2.49	0.47
1:E:35:GLY:HA3	1:E:39:GLN:O	2.15	0.47
1:F:183:ARG:NE	1:F:315:GLU:OE2	2.48	0.47
1:F:259:GLN:HA	1:F:263:ASN:HA	1.96	0.47
1:A:189:LEU:HD12	1:A:295:VAL:HG13	1.96	0.47
1:C:7:LEU:CB	1:C:8:ARG:HH21	2.27	0.47
1:D:179:ARG:HA	1:D:197:ILE:O	2.15	0.47
1:F:254:ARG:NH1	1:F:280:VAL:HG13	2.30	0.47
1:F:264:LYS:HB2	1:F:264:LYS:HE3	1.47	0.47
1:A:82:LEU:HA	1:B:60:GLN:HG3	1.96	0.47
1:A:135:HIS:HB2	1:A:220:ASP:OD2	2.15	0.47
1:C:251:PRO:HD2	1:C:254:ARG:HE	1.79	0.47
1:C:261:THR:OG1	1:C:264:LYS:HG2	2.15	0.47
1:D:229:MET:HG2	1:D:267:VAL:O	2.15	0.47
1:D:238:VAL:HG22	1:D:238:VAL:O	2.14	0.47
1:B:247:ILE:HG13	1:B:276:LEU:O	2.15	0.47
1:D:227:GLU:OE1	1:D:271:PRO:HD2	2.14	0.47
1:E:294:GLU:HG3	1:E:295:VAL:N	2.30	0.47
1:B:44:TRP:CZ2	1:B:138:PRO:HD3	2.50	0.47
1:C:295:VAL:O	1:C:299:VAL:HG23	2.15	0.46
1:A:195:ALA:HA	1:A:284:VAL:HA	1.96	0.46
1:C:201:LEU:HD13	1:C:243:VAL:HG11	1.96	0.46
1:E:230:TYR:HB3	1:E:266:ILE:CG1	2.45	0.46
1:A:247:ILE:HD12	1:A:274:GLU:HG2	1.97	0.46
1:B:84:PRO:O	1:B:88:THR:HG23	2.15	0.46
1:C:7:LEU:HD12	1:C:7:LEU:HA	1.73	0.46
1:D:261:THR:O	1:D:264:LYS:HE2	2.16	0.46
1:B:7:LEU:HA	1:B:7:LEU:HD23	1.53	0.46
1:B:186:TRP:CD2	1:B:295:VAL:HG11	2.51	0.46
1:F:185:THR:OG1	1:F:313:THR:HB	2.16	0.46
1:B:101:TYR:O	1:B:105:VAL:HG23	2.15	0.46
1:C:228:SER:HA	1:C:268:GLN:HA	1.97	0.46
1:E:98:LEU:HD11	1:E:126:VAL:HG13	1.98	0.46
1:F:189:LEU:HD13	1:F:295:VAL:HG12	1.98	0.46
1:C:181:PRO:HB2	1:C:317:LEU:HB2	1.98	0.46
1:F:76:LEU:HD11	1:F:109:ALA:H	1.81	0.46
1:C:186:TRP:HA	1:C:311:TRP:O	2.16	0.45
1:F:186:TRP:CZ3	1:F:193:VAL:HG13	2.48	0.45
1:F:197:ILE:HG21	1:F:210:LEU:HD11	1.97	0.45
1:E:53:ASP:OD1	1:F:50:ILE:HG12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:96:PRO:O	1:F:100:GLU:HG2	2.17	0.45
1:F:184:LEU:O	1:F:192:GLN:HA	2.16	0.45
1:C:76:LEU:HB3	1:C:80:ARG:CZ	2.46	0.45
1:F:72:VAL:HA	1:F:75:LEU:HD12	1.98	0.45
1:F:54:TYR:CE2	1:F:98:LEU:HD21	2.50	0.45
1:F:286:ASP:HA	1:F:289:ALA:HB3	1.98	0.45
1:A:216:THR:HA	1:A:312:LEU:O	2.17	0.45
1:C:170:VAL:HA	1:C:173:LEU:HB2	1.98	0.45
1:D:301:GLU:O	1:D:306:SER:N	2.47	0.45
1:F:34:PRO:HB2	1:F:43:ALA:CB	2.45	0.45
1:B:247:ILE:HG23	1:B:256:ARG:NH2	2.31	0.45
1:E:88:THR:HG1	1:F:276:LEU:HD21	1.82	0.45
1:F:18:GLU:CD	1:F:23:ARG:HE	2.20	0.45
1:E:44:TRP:HZ2	1:E:136:TYR:O	2.00	0.45
1:F:136:TYR:HA	1:F:307:LYS:HD2	1.99	0.45
1:A:219:GLN:HE22	1:A:312:LEU:HD22	1.82	0.44
1:A:219:GLN:NE2	1:A:231:ALA:HB2	2.32	0.44
1:F:82:LEU:HD23	1:F:82:LEU:O	2.18	0.44
1:C:257:PHE:HD1	1:C:281:LEU:HD22	1.83	0.44
1:C:85:ILE:HD11	1:D:260:ALA:HB1	2.00	0.44
1:E:236:VAL:HA	1:E:263:ASN:ND2	2.33	0.44
1:F:39:GLN:HE22	1:F:42:THR:HG23	1.82	0.44
1:A:184:LEU:O	1:A:192:GLN:HA	2.18	0.44
1:C:115:LEU:HD12	1:C:118:ARG:HD2	1.99	0.44
1:D:227:GLU:OE1	1:D:270:GLY:HA3	2.17	0.44
1:E:261:THR:HB	1:E:264:LYS:HE3	1.99	0.44
1:D:186:TRP:HZ3	1:D:193:VAL:HG22	1.83	0.44
1:D:186:TRP:HE1	1:D:219:GLN:HG2	1.83	0.44
1:F:36:SER:O	1:F:39:GLN:HG3	2.18	0.44
1:C:7:LEU:O	1:C:11:ILE:HG13	2.17	0.44
1:A:23:ARG:NH1	1:A:26:ARG:HH21	2.16	0.43
1:D:101:TYR:CD1	1:D:104:ARG:HD3	2.52	0.43
1:D:183:ARG:HD2	1:D:192:GLN:HG2	2.00	0.43
1:C:64:LEU:HB3	1:C:75:LEU:HD21	2.01	0.43
1:E:40:TYR:O	1:E:44:TRP:HB2	2.19	0.43
1:E:201:LEU:HD23	1:E:243:VAL:HG11	1.99	0.43
1:F:114:GLU:O	1:F:118:ARG:HG3	2.18	0.43
1:A:224:VAL:HA	1:B:35:GLY:HA2	2.00	0.43
1:B:30:VAL:HB	1:B:34:PRO:HD2	1.99	0.43
1:E:187:GLN:HG2	1:E:188:PRO:HA	2.00	0.43
1:B:247:ILE:HD12	1:B:274:GLU:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:117:ASP:O	1:F:121:THR:HG23	2.18	0.43
1:F:180:ILE:HG21	1:F:210:LEU:HD21	2.01	0.43
1:B:250:ALA:HB3	1:B:268:GLN:OE1	2.18	0.43
1:C:142:GLY:HA3	1:D:41:PHE:HB3	2.00	0.43
1:D:184:LEU:HD23	1:D:314:VAL:HG22	2.01	0.43
1:B:186:TRP:HZ3	1:B:193:VAL:HG13	1.84	0.43
1:C:29:THR:HG22	1:C:29:THR:O	2.17	0.43
1:C:219:GLN:NE2	1:C:231:ALA:HB2	2.34	0.43
1:D:90:LEU:HB3	1:D:95:PHE:HB2	2.01	0.43
1:E:24:ARG:HB2	1:E:29:THR:HG23	2.01	0.43
1:E:65:ALA:O	1:E:112:ARG:HD2	2.18	0.43
1:F:7:LEU:HD13	1:F:101:TYR:HD2	1.83	0.43
1:C:170:VAL:HB	1:C:201:LEU:HD11	2.00	0.43
1:C:259:GLN:HA	1:C:263:ASN:HA	1.99	0.43
1:D:7:LEU:HD12	1:D:7:LEU:HA	1.83	0.43
1:D:186:TRP:CE2	1:D:312:LEU:HD13	2.53	0.43
1:A:3:ALA:HB1	1:A:118:ARG:HG2	2.01	0.43
1:A:4:LEU:HD22	1:A:101:TYR:CD1	2.54	0.43
1:A:112:ARG:HD2	1:A:112:ARG:HA	1.93	0.43
1:D:255:LEU:HB2	1:D:282:GLY:C	2.39	0.43
1:E:247:ILE:HG23	1:E:256:ARG:CZ	2.49	0.43
1:C:36:SER:H	1:C:39:GLN:HE21	1.66	0.43
1:D:230:TYR:HB3	1:D:266:ILE:CG1	2.48	0.43
1:E:312:LEU:HD21	1:E:314:VAL:HG23	2.01	0.43
1:F:51:VAL:HG11	1:F:95:PHE:CE2	2.54	0.43
1:B:230:TYR:HB2	1:B:264:LYS:HD2	2.00	0.42
1:A:44:TRP:CZ2	1:A:138:PRO:HD3	2.54	0.42
1:E:235:LEU:HD12	1:E:237:SER:N	2.34	0.42
1:F:241:THR:HG21	1:F:279:PRO:HG3	2.01	0.42
1:E:195:ALA:HA	1:E:284:VAL:HA	2.00	0.42
1:E:235:LEU:HD11	1:E:257:PHE:CZ	2.54	0.42
1:A:210:LEU:HD23	1:A:213:LEU:HD12	2.02	0.42
1:C:219:GLN:NE2	1:C:312:LEU:HD22	2.35	0.42
1:E:81:THR:O	1:F:60:GLN:HG2	2.20	0.42
1:F:80:ARG:HA	1:F:84:PRO:HD3	2.01	0.42
1:B:204:GLN:HB2	1:B:239:ALA:HB1	2.00	0.42
1:D:170:VAL:N	1:D:173:LEU:HD13	2.35	0.42
1:D:303:THR:O	1:D:307:LYS:NZ	2.46	0.42
1:C:7:LEU:HB3	1:C:8:ARG:HH21	1.85	0.42
1:D:65:ALA:HA	1:D:75:LEU:CD2	2.47	0.42
1:F:18:GLU:HB3	1:F:23:ARG:HH21	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:GLN:CB	1:B:239:ALA:HB1	2.50	0.42
1:D:185:THR:HG23	1:D:313:THR:HB	2.02	0.42
1:E:85:ILE:HD11	1:F:261:THR:HB	2.01	0.42
1:E:187:GLN:O	1:E:311:TRP:N	2.49	0.42
1:F:39:GLN:HG3	1:F:39:GLN:H	1.72	0.42
1:F:66:THR:HG22	1:F:116:LEU:HD11	2.02	0.42
1:F:254:ARG:HD3	1:F:255:LEU:N	2.35	0.42
1:D:241:THR:OG1	1:D:244:ARG:HD2	2.20	0.41
1:B:61:LEU:HD23	1:B:64:LEU:HD12	2.01	0.41
1:C:230:TYR:HD2	1:C:266:ILE:HD12	1.85	0.41
1:E:246:ARG:NE	1:E:248:CYS:SG	2.93	0.41
1:A:186:TRP:CE2	1:A:295:VAL:HG11	2.56	0.41
1:A:219:GLN:HG3	1:A:299:VAL:HG11	2.01	0.41
1:D:192:GLN:C	1:D:291:ARG:HH22	2.22	0.41
1:A:78:VAL:HG21	1:B:78:VAL:HG11	2.02	0.41
1:A:79:PHE:O	1:A:83:ASP:HB3	2.21	0.41
1:B:213:LEU:HD22	1:B:314:VAL:O	2.21	0.41
1:B:216:THR:HA	1:B:312:LEU:O	2.20	0.41
1:B:230:TYR:HB3	1:B:266:ILE:HG13	2.02	0.41
1:F:74:ASN:HD22	1:F:74:ASN:HA	1.62	0.41
1:A:44:TRP:CH2	1:A:138:PRO:HD3	2.56	0.41
1:B:213:LEU:HD12	1:B:316:ARG:HG2	2.03	0.41
1:C:253:GLY:HA2	1:C:292:LEU:CD1	2.51	0.41
1:E:139:TRP:HD1	1:E:303:THR:O	2.03	0.41
1:A:11:ILE:O	1:A:15:VAL:HG13	2.20	0.41
1:A:60:GLN:HB2	1:B:82:LEU:HG	2.01	0.41
1:A:83:ASP:OD1	1:A:102:ALA:HB1	2.19	0.41
1:A:125:TYR:CZ	1:A:129:LEU:HD11	2.55	0.41
1:B:59:TYR:OH	1:B:259:GLN:HB3	2.20	0.41
1:E:57:ASN:ND2	1:E:86:TYR:CE2	2.89	0.41
1:E:250:ALA:HB1	1:E:254:ARG:HG2	2.02	0.41
1:A:44:TRP:HZ2	1:A:136:TYR:O	2.03	0.41
1:D:253:GLY:HA2	1:D:292:LEU:HD23	2.02	0.41
1:E:7:LEU:HD21	1:E:101:TYR:CE2	2.55	0.41
1:E:52:ARG:HH11	1:E:52:ARG:HD3	1.67	0.41
1:E:308:GLU:HA	1:E:309:PRO:HD3	1.97	0.41
1:F:248:CYS:HB2	1:F:274:GLU:O	2.20	0.41
1:A:178:GLN:HG3	1:A:200:ASP:HB3	2.03	0.41
1:B:24:ARG:HB2	1:B:29:THR:HB	2.03	0.41
1:C:92:TYR:CE1	1:D:274:GLU:HA	2.56	0.41
1:D:44:TRP:CH2	1:D:138:PRO:HD3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:131:ALA:HB2	1:D:232:TRP:CG	2.56	0.41
1:F:255:LEU:CD1	1:F:284:VAL:HG23	2.51	0.41
1:F:268:GLN:NE2	1:F:272:THR:HG21	2.35	0.41
1:F:276:LEU:HA	1:F:276:LEU:HD23	1.67	0.41
1:A:6:GLU:HB2	1:A:101:TYR:OH	2.21	0.41
1:B:135:HIS:CG	1:B:218:LEU:HD21	2.56	0.41
1:D:83:ASP:N	1:D:84:PRO:HD2	2.36	0.41
1:C:308:GLU:HA	1:C:309:PRO:HD3	1.92	0.40
1:D:19:PRO:HA	1:D:20:PRO:HD3	1.99	0.40
1:D:232:TRP:CE2	1:D:264:LYS:HD3	2.56	0.40
1:F:21:GLU:HG3	1:F:24:ARG:NH2	2.35	0.40
1:F:131:ALA:HB2	1:F:232:TRP:CG	2.55	0.40
1:A:61:LEU:HD13	1:A:79:PHE:CD1	2.49	0.40
1:B:233:ALA:HA	1:B:234:PRO:HD3	1.90	0.40
1:D:67:ASP:O	1:D:112:ARG:NH1	2.54	0.40
1:E:42:THR:HB	1:F:223:VAL:HB	2.02	0.40
1:E:98:LEU:HD23	1:E:122:PHE:HZ	1.86	0.40
1:E:194:ASP:O	1:E:285:VAL:HG12	2.21	0.40
1:E:269:TYR:CE2	1:E:296:GLY:HA3	2.56	0.40
1:A:90:LEU:HD22	1:A:95:PHE:CD2	2.57	0.40
1:A:202:ASN:HB3	1:A:205:LEU:HB3	2.04	0.40
1:B:8:ARG:HA	1:B:11:ILE:HD12	2.04	0.40
1:C:90:LEU:HA	1:C:90:LEU:HD23	1.77	0.40
1:F:23:ARG:CD	1:F:26:ARG:HH21	2.35	0.40
1:F:51:VAL:HG12	1:F:90:LEU:HD13	2.03	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	289/317 (91%)	272 (94%)	17 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	281/317 (89%)	274 (98%)	7 (2%)	0	100	100
1	C	288/317 (91%)	271 (94%)	17 (6%)	0	100	100
1	D	280/317 (88%)	267 (95%)	13 (5%)	0	100	100
1	E	282/317 (89%)	268 (95%)	14 (5%)	0	100	100
1	F	275/317 (87%)	255 (93%)	20 (7%)	0	100	100
All	All	1695/1902 (89%)	1607 (95%)	88 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 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	252/268 (94%)	236 (94%)	16 (6%)	15	35
1	B	248/268 (92%)	233 (94%)	15 (6%)	16	37
1	C	252/268 (94%)	228 (90%)	24 (10%)	7	19
1	D	247/268 (92%)	233 (94%)	14 (6%)	17	39
1	E	247/268 (92%)	235 (95%)	12 (5%)	21	45
1	F	243/268 (91%)	219 (90%)	24 (10%)	6	18
All	All	1489/1608 (93%)	1384 (93%)	105 (7%)	12	31

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	52	ARG
1	A	53	ASP
1	A	83	ASP
1	A	85	ILE
1	A	87	SER
1	A	112	ARG
1	A	114	GLU

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Mol	Chain	Res	Type
1	A	115	LEU
1	A	116	LEU
1	A	178	GLN
1	A	179	ARG
1	A	230	TYR
1	A	235	LEU
1	A	254	ARG
1	A	305	SER
1	B	1	MET
1	B	6	GLU
1	B	30	VAL
1	B	67	ASP
1	B	175	ASP
1	B	177	SER
1	B	179	ARG
1	B	194	ASP
1	B	208	ASP
1	B	230	TYR
1	B	235	LEU
1	B	286	ASP
1	B	301	GLU
1	B	306	SER
1	B	307	LYS
1	C	8	ARG
1	C	15	VAL
1	C	51	VAL
1	C	53	ASP
1	C	77	THR
1	C	82	LEU
1	C	83	ASP
1	C	85	ILE
1	C	86	TYR
1	C	92	TYR
1	C	93	ASN
1	C	145	ARG
1	C	171	ASP
1	C	179	ARG
1	C	200	ASP
1	C	235	LEU
1	C	245	GLU
1	C	247	ILE
1	C	249	ASP

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Mol	Chain	Res	Type
1	C	252	VAL
1	C	254	ARG
1	C	257	PHE
1	C	295	VAL
1	C	305	SER
1	D	30	VAL
1	D	87	SER
1	D	92	TYR
1	D	112	ARG
1	D	114	GLU
1	D	179	ARG
1	D	185	THR
1	D	215	PHE
1	D	218	LEU
1	D	230	TYR
1	D	235	LEU
1	D	246	ARG
1	D	254	ARG
1	D	286	ASP
1	E	72	VAL
1	E	92	TYR
1	E	187	GLN
1	E	194	ASP
1	E	200	ASP
1	E	216	THR
1	E	224	VAL
1	E	230	TYR
1	E	236	VAL
1	E	286	ASP
1	E	304	PHE
1	E	312	LEU
1	F	29	THR
1	F	30	VAL
1	F	33	LEU
1	F	36	SER
1	F	39	GLN
1	F	71	SER
1	F	72	VAL
1	F	74	ASN
1	F	77	THR
1	F	83	ASP
1	F	92	TYR

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Mol	Chain	Res	Type
1	F	97	VAL
1	F	133	SER
1	F	230	TYR
1	F	235	LEU
1	F	258	SER
1	F	259	GLN
1	F	264	LYS
1	F	265	VAL
1	F	283	LYS
1	F	286	ASP
1	F	287	SER
1	F	290	ASP
1	F	291	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	178	GLN
1	A	219	GLN
1	B	74	ASN
1	C	219	GLN
1	D	103	GLN
1	E	57	ASN
1	F	39	GLN
1	F	259	GLN
1	F	268	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

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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	293/317 (92%)	-1.88	0 100 100	16, 31, 50, 75	0
1	B	287/317 (90%)	-1.89	0 100 100	21, 35, 50, 75	0
1	C	292/317 (92%)	-1.81	0 100 100	28, 46, 62, 74	0
1	D	284/317 (89%)	-1.78	0 100 100	35, 45, 63, 86	0
1	E	286/317 (90%)	-1.72	0 100 100	31, 55, 79, 96	0
1	F	279/317 (88%)	-1.75	0 100 100	29, 54, 75, 97	0
All	All	1721/1902 (90%)	-1.81	0 100 100	16, 45, 69, 97	0

There are no RSRZ outliers to report.

### 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 monosaccharides 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.