



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 09:44 pm GMT

PDB ID : 3VLB  
Title : Crystal structure of xeg-edgp  
Authors : Yoshizawa, T.; Shimizu, T.; Hirano, H.; Sato, M.; Hashimoto, H.  
Deposited on : 2011-11-30  
Resolution : 2.70 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

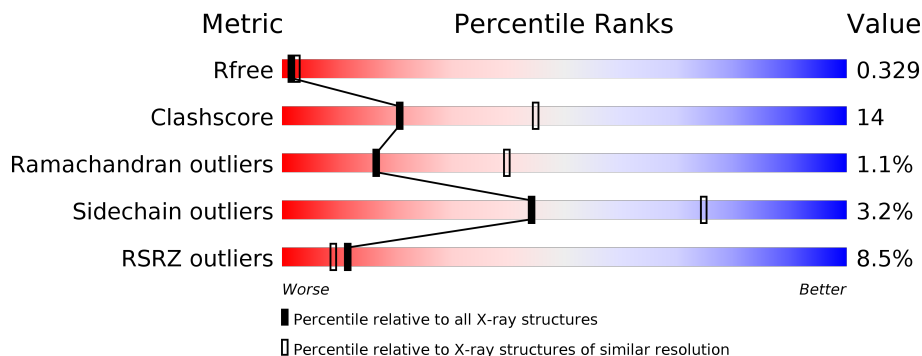
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	413	
1	C	413	
2	B	222	
2	D	222	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9285 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 EDGP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	404	Total	C	N	O	S	1	0	0
			2991	1876	506	594	15			
1	C	403	Total	C	N	O	S	0	0	0
			2985	1873	504	593	15			

- Molecule 2 is a protein called Xyloglucan-specific endo-beta-1,4-glucanase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	218	Total	C	N	O	S	0	0	0
			1628	1028	245	351	4			
2	D	218	Total	C	N	O	S	1	0	0
			1628	1028	245	351	4			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	3	GLY	-	EXPRESSION TAG	UNP O94218
B	4	PRO	-	EXPRESSION TAG	UNP O94218
B	5	LEU	-	EXPRESSION TAG	UNP O94218
B	6	GLY	-	EXPRESSION TAG	UNP O94218
D	3	GLY	-	EXPRESSION TAG	UNP O94218
D	4	PRO	-	EXPRESSION TAG	UNP O94218
D	5	LEU	-	EXPRESSION TAG	UNP O94218
D	6	GLY	-	EXPRESSION TAG	UNP O94218

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	17	Total	O	0	0
			17	17		
3	B	11	Total	O	0	0
			11	11		

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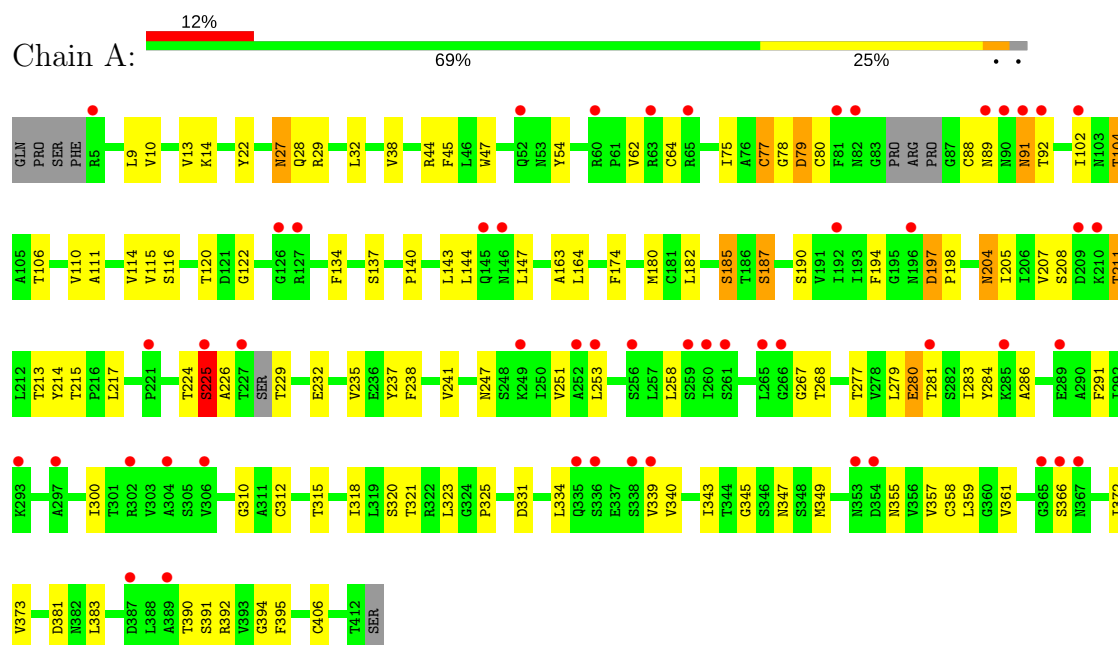
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	14	Total	O	0	0
			14	14		
3	D	11	Total	O	0	0
			11	11		

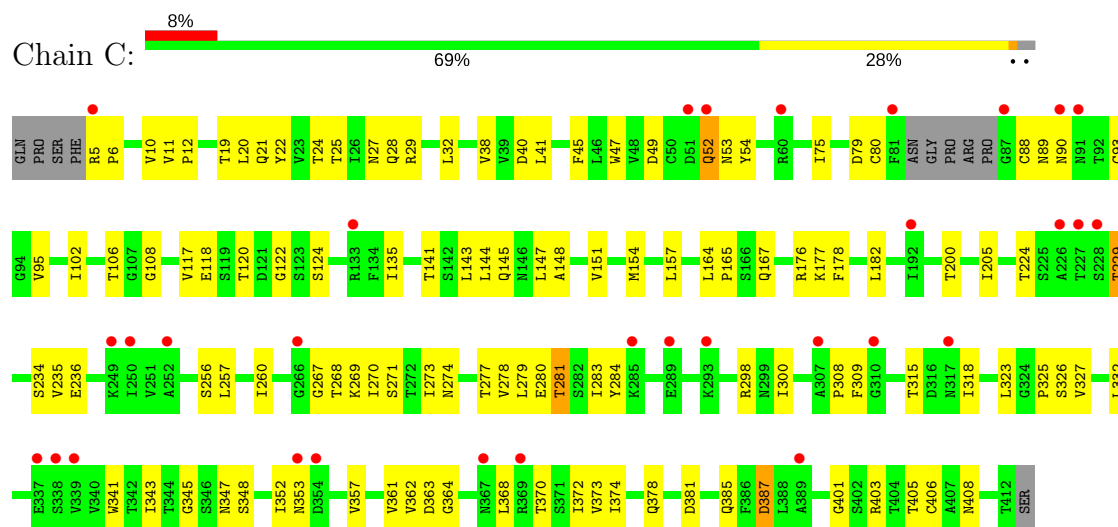
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

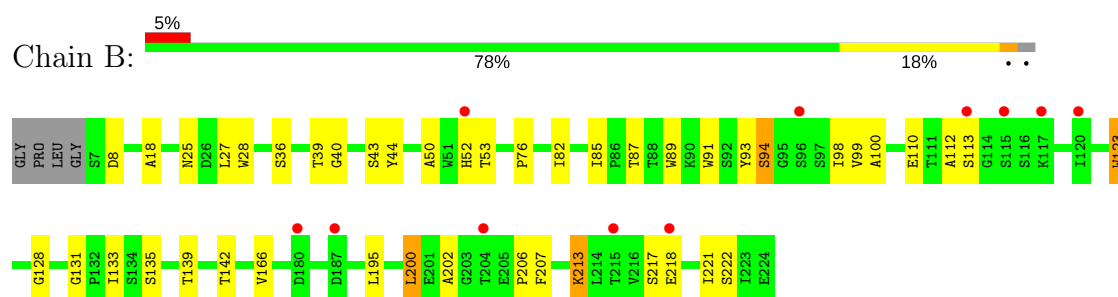
#### • Molecule 1: EDGP



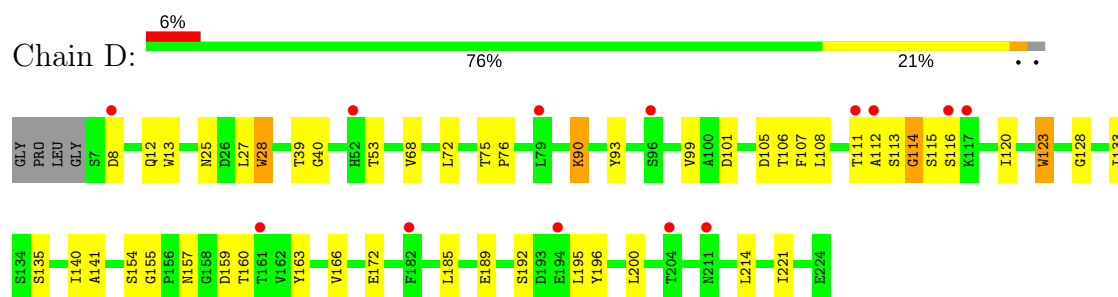
#### • Molecule 1: EDGP



#### • Molecule 2: Xyloglucan-specific endo-beta-1,4-glucanase A



• Molecule 2: Xyloglucan-specific endo-beta-1,4-glucanase A



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	249.04Å 51.69Å 143.24Å 90.00° 122.21° 90.00°	Depositor
Resolution (Å)	10.00 – 2.70 19.98 – 2.70	Depositor EDS
% Data completeness (in resolution range)	92.0 (10.00-2.70) 92.0 (19.98-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.21 (at 2.71Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.257 , 0.341 0.253 , 0.329	Depositor DCC
$R_{free}$ test set	1983 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	59.7	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 34.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.076 for -h-2*k,l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	9285	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% 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	0.70	2/3039 (0.1%)	0.79	0/4141
1	C	0.69	1/3034 (0.0%)	0.78	0/4136
2	B	0.83	3/1672 (0.2%)	0.77	0/2292
2	D	0.86	3/1672 (0.2%)	0.79	3/2292 (0.1%)
All	All	0.75	9/9417 (0.1%)	0.79	3/12861 (0.0%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	90	LYS	CE-NZ	-8.69	1.27	1.49
1	A	27	ASN	CG-ND2	8.09	1.53	1.32
2	D	28	TRP	CD2-CE2	7.75	1.50	1.41
2	D	123	TRP	CD2-CE2	7.12	1.49	1.41
2	B	123	TRP	CD2-CE2	5.72	1.48	1.41
2	B	91	TRP	CD2-CE2	5.54	1.48	1.41
2	B	28	TRP	CD2-CE2	5.35	1.47	1.41
1	A	225	SER	CA-CB	5.16	1.60	1.52
1	C	47	TRP	CD2-CE2	5.04	1.47	1.41

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	D	101	ASP	CB-CG-OD1	6.71	124.34	118.30
2	D	101	ASP	CB-CG-OD2	-5.22	113.60	118.30
2	D	105	ASP	CB-CG-OD2	-5.22	113.60	118.30

There are no chirality outliers.

There are no planarity outliers.



## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2991	0	2986	102	0
1	C	2985	0	2983	93	0
2	B	1628	0	1487	34	0
2	D	1628	0	1487	30	0
3	A	17	0	0	0	0
3	B	11	0	0	2	0
3	C	14	0	0	1	0
3	D	11	0	0	0	0
All	All	9285	0	8943	250	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 (250) 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:120:THR:HG22	1:C:122:GLY:H	1.10	1.10
1:C:11:VAL:HG12	1:C:117:VAL:HG11	1.31	1.09
1:A:64:CYS:HB3	1:A:91:ASN:HB3	1.39	1.03
1:A:349:MET:HE3	1:A:357:VAL:HG12	1.48	0.95
1:C:300:ILE:HD13	1:C:318:ILE:HD13	1.49	0.94
1:C:277:THR:O	1:C:361:VAL:HG13	1.67	0.94
1:A:349:MET:CE	1:A:357:VAL:HG12	2.01	0.91
1:C:11:VAL:CG1	1:C:117:VAL:HG11	2.05	0.87
1:C:27:ASN:HB3	1:C:32:LEU:HD12	1.63	0.81
2:B:142:THR:CG2	3:B:234:HOH:O	2.29	0.80
1:C:38:VAL:HG21	1:C:147:LEU:HD22	1.64	0.80
1:C:279:LEU:HG	1:C:361:VAL:HG11	1.63	0.79
1:C:11:VAL:HG12	1:C:117:VAL:CG1	2.12	0.78
2:B:142:THR:HG22	3:B:234:HOH:O	1.83	0.78
1:A:78:GLY:H	1:A:92:THR:H	1.31	0.78
1:A:38:VAL:HG21	1:A:147:LEU:HD22	1.67	0.77
1:C:75:ILE:HD13	1:C:229:THR:HG23	1.67	0.76
1:C:120:THR:HG22	1:C:122:GLY:N	1.96	0.76
1:A:390:THR:HB	1:A:392:ARG:NH1	2.01	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:ILE:HD12	1:C:167:GLN:OE1	1.86	0.75
1:A:29:ARG:O	1:A:32:LEU:HD12	1.87	0.74
1:C:300:ILE:HD13	1:C:318:ILE:CD1	2.17	0.73
1:A:253:LEU:HD22	1:A:283:ILE:HA	1.68	0.73
1:A:64:CYS:CB	1:A:91:ASN:HB3	2.19	0.72
2:D:106:THR:HG22	2:D:200:LEU:HD23	1.71	0.72
1:A:229:THR:HG22	1:A:232:GLU:HB2	1.71	0.71
1:C:120:THR:HG23	1:C:124:SER:O	1.90	0.70
1:C:12:PRO:O	1:C:24:THR:HG23	1.90	0.70
1:A:44:ARG:HG2	1:A:235:VAL:HG21	1.74	0.70
1:A:349:MET:HE3	1:A:357:VAL:CG1	2.22	0.70
1:A:229:THR:CG2	1:A:232:GLU:HB2	2.22	0.70
2:D:185:LEU:HD23	2:D:189:GLU:HG3	1.76	0.67
1:A:253:LEU:CD2	1:A:283:ILE:HA	2.24	0.67
2:B:200:LEU:HD22	2:B:221:ILE:HD13	1.76	0.67
1:A:106:THR:HG22	1:A:143:LEU:HD13	1.76	0.66
1:A:349:MET:CE	1:A:357:VAL:CG1	2.73	0.66
1:A:277:THR:HG23	1:A:373:VAL:O	1.94	0.66
1:A:300:ILE:HD13	1:A:318:ILE:HD13	1.77	0.66
1:C:273:ILE:HD12	1:C:274:ASN:N	2.11	0.65
1:A:22:TYR:CD1	1:A:182:LEU:HD22	2.33	0.64
1:C:279:LEU:HD13	1:C:283:ILE:HG22	1.80	0.64
1:C:257:LEU:HD13	1:C:283:ILE:HD11	1.80	0.63
1:C:52:GLN:O	1:C:54:TYR:N	2.26	0.63
1:A:10:VAL:HG12	1:A:120:THR:HG23	1.80	0.62
1:A:180:MET:HE3	1:A:182:LEU:HD11	1.81	0.62
1:A:279:LEU:HD22	1:A:361:VAL:HG11	1.80	0.62
1:C:89:ASN:OD1	1:C:90:ASN:N	2.33	0.62
1:A:79:ASP:HB2	1:A:92:THR:HG21	1.80	0.61
1:A:77:CYS:SG	1:A:91:ASN:CG	2.79	0.61
2:B:217:SER:O	2:B:218:GLU:HG3	2.00	0.60
1:C:141:THR:O	1:C:144:LEU:HD23	2.00	0.60
2:B:94:SER:O	2:B:98:ILE:HD11	2.01	0.60
1:C:75:ILE:CD1	1:C:229:THR:HG23	2.32	0.60
1:C:205:ILE:N	1:C:205:ILE:HD12	2.17	0.59
1:A:10:VAL:CG1	1:A:120:THR:HG23	2.32	0.59
1:A:320:SER:HB3	2:B:207:PHE:CE2	2.38	0.59
1:C:271:SER:HB2	3:C:425:HOH:O	2.02	0.59
1:A:10:VAL:HB	1:A:120:THR:HG21	1.85	0.58
1:A:253:LEU:HD21	1:A:286:ALA:HB3	1.84	0.58
2:D:106:THR:CG2	2:D:200:LEU:HD23	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:LEU:O	1:A:267:GLY:HA2	2.04	0.58
1:A:291:PHE:CE2	1:A:359:LEU:HD13	2.39	0.58
1:C:403:ARG:HG3	2:D:28:TRP:CE2	2.38	0.58
1:A:208:SER:O	1:A:211:THR:HG22	2.04	0.57
1:A:10:VAL:HG13	1:A:10:VAL:O	2.03	0.57
1:C:106:THR:HG22	1:C:143:LEU:HD13	1.86	0.57
1:A:390:THR:HG22	1:A:390:THR:O	2.05	0.57
1:A:213:THR:O	1:A:394:GLY:HA2	2.05	0.56
1:C:298:ARG:NH2	2:D:135:SER:O	2.38	0.56
1:A:120:THR:HB	1:A:122:GLY:H	1.70	0.56
1:A:253:LEU:CD2	1:A:286:ALA:HB3	2.36	0.56
1:A:300:ILE:HD13	1:A:318:ILE:CD1	2.35	0.56
1:A:79:ASP:CB	1:A:92:THR:HG21	2.36	0.55
1:A:144:LEU:HA	1:A:147:LEU:HD12	1.88	0.55
1:C:141:THR:HA	1:C:144:LEU:HD23	1.88	0.55
1:A:27:ASN:HB2	1:A:116:SER:O	2.06	0.55
1:C:41:LEU:HD23	1:C:270:ILE:O	2.07	0.55
2:D:116:SER:O	2:D:160:THR:HG22	2.07	0.54
1:A:185:SER:OG	1:A:187:SER:N	2.40	0.54
1:C:260:ILE:N	1:C:260:ILE:HD13	2.22	0.54
1:A:331:ASP:HB3	1:A:340:VAL:HG11	1.89	0.54
1:C:10:VAL:O	1:C:10:VAL:HG13	2.07	0.54
1:A:62:VAL:HG21	1:A:110:VAL:HG12	1.90	0.54
1:C:49:ASP:HB2	1:C:144:LEU:HD21	1.90	0.54
1:C:257:LEU:CD1	1:C:283:ILE:HD11	2.38	0.54
1:C:278:VAL:O	1:C:279:LEU:HD23	2.08	0.53
1:A:390:THR:HB	1:A:392:ARG:HH11	1.71	0.53
1:C:361:VAL:HG12	1:C:362:VAL:N	2.22	0.53
1:A:77:CYS:SG	1:A:91:ASN:OD1	2.65	0.53
1:C:300:ILE:HG21	1:C:318:ILE:HD11	1.91	0.53
2:B:200:LEU:CD2	2:B:221:ILE:CD1	2.87	0.53
1:C:205:ILE:N	1:C:205:ILE:CD1	2.71	0.53
2:B:142:THR:HG22	2:B:142:THR:O	2.08	0.53
2:B:43:SER:OG	2:B:50:ALA:HB3	2.08	0.52
1:A:325:PRO:HD2	1:A:345:GLY:HA3	1.90	0.52
1:A:349:MET:HE2	1:A:357:VAL:CG1	2.39	0.52
2:B:25:ASN:O	2:B:27:LEU:HD23	2.10	0.52
1:A:75:ILE:HD11	1:A:229:THR:OG1	2.08	0.52
2:B:200:LEU:HD22	2:B:221:ILE:CD1	2.38	0.52
2:D:111:THR:HG22	2:D:112:ALA:N	2.25	0.52
1:C:147:LEU:HD21	1:C:154:MET:CE	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:ASP:O	1:A:89:ASN:N	2.31	0.51
1:A:106:THR:HG21	1:A:140:PRO:HD2	1.92	0.51
1:A:207:VAL:HG11	1:A:383:LEU:HD22	1.92	0.51
1:A:215:THR:HB	1:A:334:LEU:HD13	1.92	0.51
1:C:284:TYR:CE2	1:C:363:ASP:HB2	2.45	0.51
1:C:147:LEU:HD21	1:C:154:MET:HE2	1.93	0.51
1:C:102:ILE:HD13	1:C:145:GLN:HB3	1.93	0.51
1:A:312:CYS:HA	1:A:358:CYS:HA	1.92	0.50
1:C:268:THR:HA	1:C:372:ILE:O	2.11	0.50
1:C:106:THR:CG2	1:C:143:LEU:HD13	2.41	0.50
1:C:300:ILE:CD1	1:C:318:ILE:HD13	2.30	0.50
1:A:204:ASN:ND2	1:A:205:ILE:HD13	2.26	0.50
1:C:144:LEU:HA	1:C:147:LEU:HD12	1.93	0.50
1:A:284:TYR:OH	1:A:310:GLY:HA3	2.11	0.50
1:A:78:GLY:N	1:A:91:ASN:HA	2.26	0.50
1:A:92:THR:O	1:A:92:THR:HG23	2.12	0.50
1:C:144:LEU:HD22	1:C:144:LEU:N	2.26	0.50
1:C:277:THR:HG23	1:C:374:ILE:HA	1.94	0.50
2:D:140:ILE:O	2:D:141:ALA:HB2	2.12	0.50
2:B:82:ILE:HD13	2:B:85:ILE:HD11	1.94	0.49
1:C:117:VAL:HG12	1:C:118:GLU:H	1.77	0.49
1:C:224:THR:HG22	1:C:224:THR:O	2.11	0.49
2:D:72:LEU:HD22	2:D:221:ILE:HG23	1.95	0.49
1:C:357:VAL:O	1:C:357:VAL:HG13	2.12	0.49
1:C:277:THR:HG23	1:C:373:VAL:O	2.12	0.49
1:A:197:ASP:HB2	1:A:198:PRO:HA	1.94	0.49
1:C:284:TYR:CD2	1:C:363:ASP:HB2	2.48	0.49
1:A:102:ILE:HD12	1:A:104:THR:OG1	2.12	0.48
1:A:229:THR:HG21	1:A:232:GLU:CG	2.44	0.48
1:C:300:ILE:CG2	1:C:318:ILE:HD11	2.43	0.48
1:A:349:MET:HE2	1:A:357:VAL:HG12	1.89	0.48
1:A:315:THR:HG22	1:A:357:VAL:HG23	1.94	0.48
1:A:79:ASP:CG	1:A:92:THR:HG21	2.34	0.48
1:A:323:LEU:HD12	2:B:133:ILE:HG12	1.95	0.48
2:B:99:VAL:HG22	2:B:128:GLY:O	2.12	0.48
2:B:200:LEU:HD21	2:B:221:ILE:HD11	1.94	0.48
1:C:224:THR:O	1:C:224:THR:CG2	2.61	0.48
2:B:39:THR:HG22	2:B:40:GLY:N	2.28	0.47
2:D:192:SER:HB3	2:D:195:LEU:HG	1.96	0.47
1:A:214:TYR:CE1	1:A:394:GLY:HA3	2.49	0.47
1:A:241:VAL:CG2	1:A:258:LEU:HD22	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:VAL:HG23	1:A:111:ALA:HA	1.96	0.47
1:C:177:LYS:HD3	1:C:385:GLN:OE1	2.15	0.47
1:C:361:VAL:CG1	1:C:362:VAL:N	2.76	0.47
2:D:123:TRP:HB2	2:D:166:VAL:HA	1.95	0.47
1:C:234:SER:OG	1:C:236:GLU:HG3	2.14	0.47
1:C:29:ARG:O	1:C:32:LEU:HD22	2.14	0.47
1:C:177:LYS:HD3	1:C:385:GLN:CD	2.35	0.47
1:A:28:GLN:HA	1:A:114:VAL:O	2.15	0.47
1:C:347:ASN:O	1:C:378:GLN:NE2	2.47	0.47
1:A:10:VAL:CG1	1:A:120:THR:CG2	2.93	0.47
2:B:53:THR:O	2:B:53:THR:HG23	2.15	0.47
1:A:283:ILE:N	1:A:283:ILE:HD12	2.30	0.47
1:A:80:CYS:HA	1:A:88:CYS:HA	1.96	0.47
2:B:25:ASN:OD1	2:B:39:THR:OG1	2.29	0.46
1:C:5:ARG:HB2	1:C:6:PRO:HD3	1.97	0.46
2:D:108:LEU:HA	2:D:196:TYR:O	2.14	0.46
1:C:279:LEU:HG	1:C:361:VAL:CG1	2.40	0.46
1:C:280:GLU:OE2	1:C:281:THR:N	2.48	0.46
2:D:25:ASN:O	2:D:68:VAL:HG22	2.15	0.46
2:B:89:TRP:CH2	2:B:202:ALA:HB1	2.50	0.46
1:A:79:ASP:OD2	1:A:92:THR:HG21	2.16	0.46
1:A:343:ILE:HG23	1:A:347:ASN:CB	2.46	0.46
1:A:47:TRP:HA	1:A:137:SER:O	2.16	0.46
1:C:381:ASP:HA	1:C:406:CYS:SG	2.56	0.46
1:A:381:ASP:HA	1:A:406:CYS:SG	2.56	0.45
2:B:200:LEU:CD2	2:B:221:ILE:HD11	2.46	0.45
2:B:52:HIS:HB2	2:B:213:LYS:HD3	1.97	0.45
2:B:18:ALA:HB1	2:B:44:TYR:CG	2.51	0.45
1:A:315:THR:OG1	1:A:355:ASN:HA	2.16	0.45
1:C:315:THR:HA	1:C:318:ILE:HG13	1.98	0.45
1:C:278:VAL:HG13	1:C:364:GLY:HA3	1.99	0.45
1:A:10:VAL:HB	1:A:120:THR:CG2	2.46	0.45
2:D:27:LEU:HD23	2:D:27:LEU:N	2.31	0.45
1:A:224:THR:O	1:A:226:ALA:N	2.49	0.45
1:A:334:LEU:HD12	1:A:339:VAL:HG12	1.98	0.45
1:C:325:PRO:O	1:C:327:VAL:N	2.50	0.44
1:A:28:GLN:O	1:A:29:ARG:HB2	2.17	0.44
1:C:343:ILE:HG23	1:C:347:ASN:HB2	1.98	0.44
1:A:106:THR:CG2	1:A:143:LEU:HD22	2.47	0.44
1:A:331:ASP:HB3	1:A:340:VAL:CG1	2.46	0.44
1:C:40:ASP:O	1:C:41:LEU:C	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:VAL:CG1	1:A:286:ALA:HB1	2.48	0.44
1:A:349:MET:HB3	1:A:357:VAL:HG13	1.99	0.44
1:C:345:GLY:HA2	1:C:348:SER:OG	2.17	0.44
2:D:12:GLN:HG2	2:D:13:TRP:CE2	2.52	0.44
1:A:115:VAL:HG23	1:A:134:PHE:HB3	2.00	0.44
1:A:204:ASN:HD22	1:A:204:ASN:C	2.21	0.44
1:C:177:LYS:HE2	1:C:387:ASP:OD1	2.18	0.44
1:A:13:VAL:HG12	1:A:14:LYS:N	2.34	0.43
1:A:9:LEU:HB2	1:A:194:PHE:HB2	2.00	0.43
1:C:19:THR:O	1:C:20:LEU:HB2	2.17	0.43
1:C:22:TYR:CD1	1:C:182:LEU:HD22	2.53	0.43
1:C:260:ILE:CD1	1:C:267:GLY:HA3	2.48	0.43
1:C:80:CYS:HA	1:C:88:CYS:HA	1.99	0.43
1:C:401:GLY:C	2:D:157:ASN:HD21	2.21	0.43
1:A:321:THR:HG22	2:B:131:GLY:O	2.18	0.43
2:B:100:ALA:HB2	2:B:206:PRO:HA	2.01	0.43
2:D:99:VAL:HG22	2:D:128:GLY:O	2.19	0.43
1:A:280:GLU:OE2	1:A:281:THR:N	2.51	0.43
2:B:100:ALA:CB	2:B:206:PRO:HA	2.48	0.43
1:A:229:THR:CG2	1:A:232:GLU:CB	2.95	0.43
1:C:405:THR:OG1	1:C:408:ASN:OD1	2.36	0.43
2:B:89:TRP:CZ3	2:B:202:ALA:HB1	2.54	0.42
1:C:24:THR:HG22	1:C:25:THR:N	2.33	0.42
1:C:352:ILE:HG23	1:C:353:ASN:N	2.34	0.42
2:D:120:ILE:HD12	2:D:120:ILE:N	2.34	0.42
1:C:403:ARG:HG3	2:D:28:TRP:CZ2	2.54	0.42
2:B:76:PRO:HB2	2:B:112:ALA:HB1	2.01	0.42
1:A:247:ASN:ND2	2:B:135:SER:O	2.47	0.42
2:B:85:ILE:HG22	2:B:85:ILE:O	2.19	0.42
1:C:148:ALA:O	1:C:151:VAL:HG22	2.19	0.42
2:D:75:THR:O	2:D:76:PRO:C	2.57	0.42
2:B:43:SER:OG	2:B:50:ALA:CB	2.67	0.42
1:A:390:THR:HB	1:A:392:ARG:HH12	1.82	0.42
1:C:323:LEU:HD11	2:D:133:ILE:HD13	2.02	0.42
1:A:213:THR:HB	1:A:395:PHE:CE2	2.55	0.42
2:B:87:THR:O	2:B:87:THR:HG23	2.19	0.42
2:D:133:ILE:HG22	2:D:155:GLY:HA3	2.01	0.42
2:D:111:THR:HB	2:D:114:GLY:H	1.85	0.41
1:A:106:THR:HG22	1:A:143:LEU:HD22	2.01	0.41
1:C:283:ILE:N	1:C:283:ILE:HD12	2.34	0.41
2:D:107:PHE:O	2:D:108:LEU:HD23	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:53:THR:HG22	2:D:214:LEU:HB3	2.01	0.41
1:A:28:GLN:O	1:A:29:ARG:CB	2.69	0.41
2:B:123:TRP:HB2	2:B:166:VAL:HA	2.00	0.41
1:C:95:VAL:N	1:C:108:GLY:O	2.40	0.41
1:C:332:LEU:HB2	1:C:341:TRP:HB3	2.00	0.41
2:D:39:THR:HG22	2:D:40:GLY:N	2.34	0.41
1:A:163:ALA:O	1:A:164:LEU:C	2.57	0.41
1:C:236:GLU:OE2	1:C:269:LYS:HE2	2.20	0.41
1:A:207:VAL:CG1	1:A:383:LEU:HD22	2.50	0.41
1:C:157:LEU:HD23	1:C:178:PHE:CE1	2.56	0.41
1:C:28:GLN:O	1:C:29:ARG:CB	2.69	0.41
2:B:85:ILE:HA	2:B:222:SER:O	2.20	0.41
1:C:10:VAL:O	1:C:10:VAL:CG1	2.69	0.41
2:D:163:TYR:CD1	2:D:185:LEU:CD2	3.04	0.41
1:A:343:ILE:HG23	1:A:347:ASN:HB3	2.02	0.41
1:C:28:GLN:O	1:C:29:ARG:HB2	2.21	0.41
2:D:90:LYS:HA	2:D:172:GLU:O	2.21	0.41
2:B:110:GLU:HG2	2:B:195:LEU:HD22	2.03	0.41
1:C:308:PRO:HD2	1:C:309:PHE:CE2	2.56	0.41
1:C:343:ILE:HG23	1:C:347:ASN:CB	2.51	0.40
1:A:217:LEU:HD11	1:A:237:TYR:HD1	1.86	0.40
1:A:238:PHE:HA	1:A:268:THR:O	2.21	0.40
1:A:268:THR:HG23	1:A:372:ILE:HG22	2.03	0.40
2:D:159:ASP:OD2	2:D:159:ASP:N	2.52	0.40
1:C:164:LEU:N	1:C:165:PRO:CD	2.84	0.40
2:D:163:TYR:CD1	2:D:185:LEU:HD22	2.56	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	398/413 (96%)	368 (92%)	26 (6%)	4 (1%)	18	43
1	C	399/413 (97%)	367 (92%)	24 (6%)	8 (2%)	9	22
2	B	216/222 (97%)	207 (96%)	8 (4%)	1 (0%)	32	60
2	D	216/222 (97%)	205 (95%)	10 (5%)	1 (0%)	32	60
All	All	1229/1270 (97%)	1147 (93%)	68 (6%)	14 (1%)	17	40

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	ASN
1	C	53	ASN
1	C	229	THR
1	C	326	SER
1	A	197	ASP
1	A	225	SER
2	D	114	GLY
2	B	113	SER
1	C	93	CYS
1	C	176	ARG
1	A	187	SER
1	C	256	SER
1	C	52	GLN
1	C	281	THR

### 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	347/356 (98%)	333 (96%)	14 (4%)	36	67
1	C	347/356 (98%)	339 (98%)	8 (2%)	56	84
2	B	178/180 (99%)	171 (96%)	7 (4%)	37	68
2	D	178/180 (99%)	173 (97%)	5 (3%)	49	79
All	All	1050/1072 (98%)	1016 (97%)	34 (3%)	44	75



All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	PHE
1	A	54	TYR
1	A	77	CYS
1	A	79	ASP
1	A	104	THR
1	A	174	PHE
1	A	185	SER
1	A	190	SER
1	A	204	ASN
1	A	211	THR
1	A	225	SER
1	A	280	GLU
1	A	366	SER
1	A	391	SER
2	B	8	ASP
2	B	36	SER
2	B	93	TYR
2	B	94	SER
2	B	139	THR
2	B	200	LEU
2	B	213	LYS
1	C	21	GLN
1	C	45	PHE
1	C	79	ASP
1	C	200	THR
1	C	235	VAL
1	C	368	LEU
1	C	370	THR
1	C	387	ASP
2	D	8	ASP
2	D	93	TYR
2	D	113	SER
2	D	115	SER
2	D	154	SER

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

Mol	Chain	Res	Type
1	A	146	ASN
1	A	204	ASN
2	B	69	ASN

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Mol	Chain	Res	Type
2	B	188	ASN
1	C	385	GLN
2	D	188	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 carbohydrates 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, 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	404/413 (97%)	0.65	51 (12%) 4 3	29, 51, 82, 106	6 (1%)
1	C	403/413 (97%)	0.58	31 (7%) 14 12	29, 52, 81, 100	4 (0%)
2	B	218/222 (98%)	0.38	11 (5%) 30 28	30, 46, 67, 86	0
2	D	218/222 (98%)	0.43	13 (5%) 23 21	29, 48, 70, 81	1 (0%)
All	All	1243/1270 (97%)	0.54	106 (8%) 11 9	29, 50, 79, 106	11 (0%)

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	91	ASN	12.3
2	D	96	SER	6.2
2	D	112	ALA	5.9
1	A	367	ASN	5.6
1	C	227	THR	5.1
1	C	337	GLU	5.1
1	A	89	ASN	5.0
1	A	266	GLY	4.9
1	C	228	SER	4.6
1	C	249	LYS	4.6
1	C	51	ASP	4.5
1	A	336	SER	4.4
2	B	96	SER	4.4
1	A	353	ASN	4.4
1	A	338	SER	4.3
1	A	52	GLN	3.9
2	B	218	GLU	3.9
1	A	256	SER	3.9
1	C	310	GLY	3.8
1	A	225	SER	3.8
1	A	127	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	81	PHE	3.7
1	A	281	THR	3.7
1	A	145	GLN	3.7
1	A	289	GLU	3.7
2	B	180	ASP	3.6
1	C	338	SER	3.6
1	A	196	ASN	3.5
1	A	389	ALA	3.5
2	D	194	GLU	3.5
1	C	293	LYS	3.5
1	C	5	ARG	3.5
1	A	339	VAL	3.4
1	A	5	ARG	3.3
2	D	161	THR	3.3
1	A	252	ALA	3.2
1	C	289	GLU	3.1
1	A	259	SER	3.0
1	A	81	PHE	3.0
1	C	353	ASN	3.0
1	A	90	ASN	2.9
1	C	252	ALA	2.9
1	C	339	VAL	2.9
1	A	260	ILE	2.9
1	A	366	SER	2.8
1	C	285	LYS	2.8
2	D	204	THR	2.8
1	A	253	LEU	2.7
2	D	79	LEU	2.7
2	D	211	ASN	2.7
1	A	365	GLY	2.7
1	A	285	LYS	2.6
1	C	60	ARG	2.6
2	B	215	THR	2.6
1	C	307	ALA	2.6
1	C	367	ASN	2.6
1	A	304	ALA	2.6
1	A	265	LEU	2.6
1	A	92	THR	2.6
1	C	250	ILE	2.5
2	B	204	THR	2.5
1	A	302	ARG	2.5
1	A	249	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	52	HIS	2.5
1	C	192	ILE	2.5
2	D	8	ASP	2.5
1	A	293	LYS	2.5
2	B	117	LYS	2.5
2	B	113	SER	2.5
2	D	117	LYS	2.4
2	D	182	PHE	2.4
1	A	63	ARG	2.4
1	A	221	PRO	2.4
2	B	120	ILE	2.4
2	B	52	HIS	2.4
1	A	209	ASP	2.4
1	A	82	ASN	2.4
1	A	65	ARG	2.4
1	A	126	GLY	2.3
1	A	210	LYS	2.3
1	C	266	GLY	2.3
1	A	192	ILE	2.3
2	B	187	ASP	2.3
1	A	261	SER	2.3
1	A	335	GLN	2.3
1	A	102	ILE	2.3
1	C	52	GLN	2.2
1	C	91	ASN	2.2
2	D	116	SER	2.2
1	A	227	THR	2.2
1	C	133	ARG	2.2
1	A	354	ASP	2.2
1	C	87	GLY	2.2
1	C	90	ASN	2.1
1	C	317	ASN	2.1
2	B	115	SER	2.1
1	A	297	ALA	2.1
1	A	146	ASN	2.1
1	A	60	ARG	2.1
2	D	111	THR	2.1
1	C	369	ARG	2.0
1	A	306	VAL	2.0
1	C	389	ALA	2.0
1	A	387	ASP	2.0
1	C	226	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	354	ASP	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.