



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:33 AM UTC

PDB ID : 2ZR3 / pdb_00002zr3
Title : Crystal structure of seryl-tRNA synthetase from *Pyrococcus horikoshii*
Authors : Itoh, Y.; Sekine, S.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2008-08-22
Resolution : 3.00 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

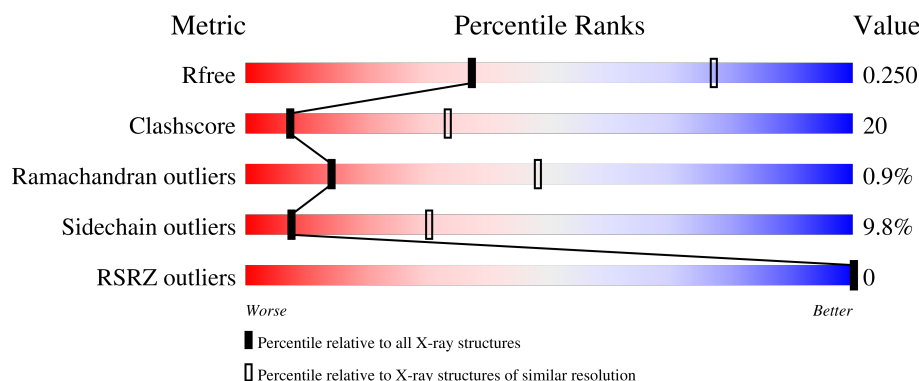
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	455	
1	B	455	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7446 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 Seryl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	448	Total	C	N	O	S	0	0	0
			3708	2382	647	671	8			
1	B	448	Total	C	N	O	S	0	0	0
			3708	2382	647	671	8			

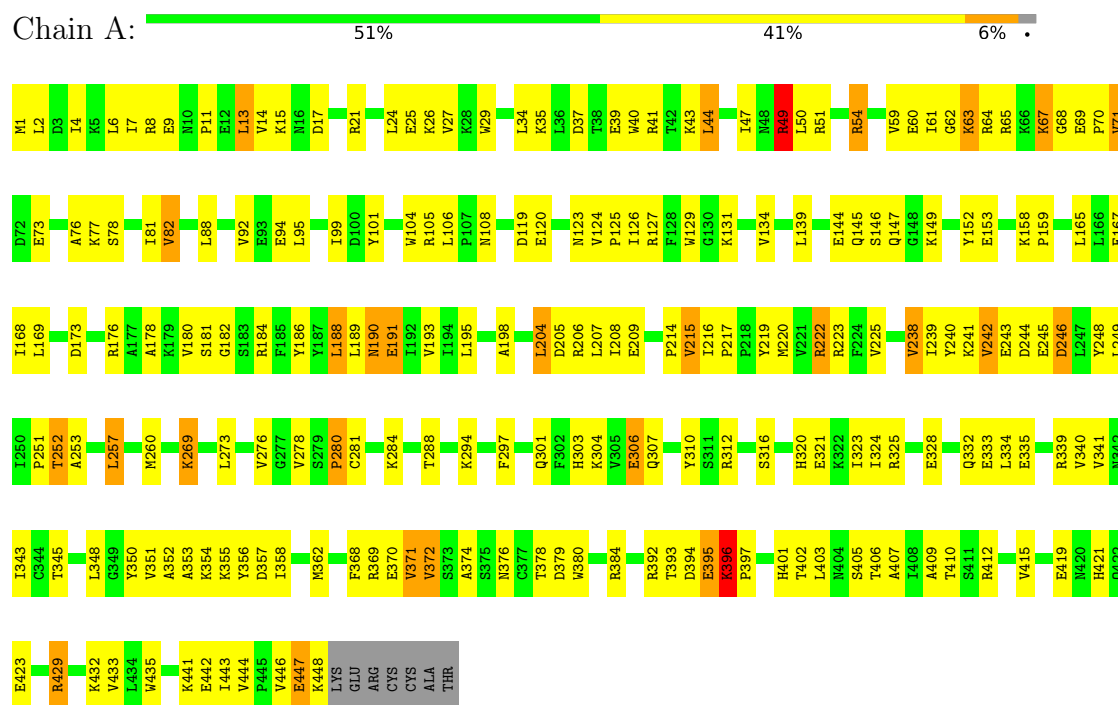
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	13	Total	O	0	0
			13	13		
2	B	17	Total	O	0	0
			17	17		

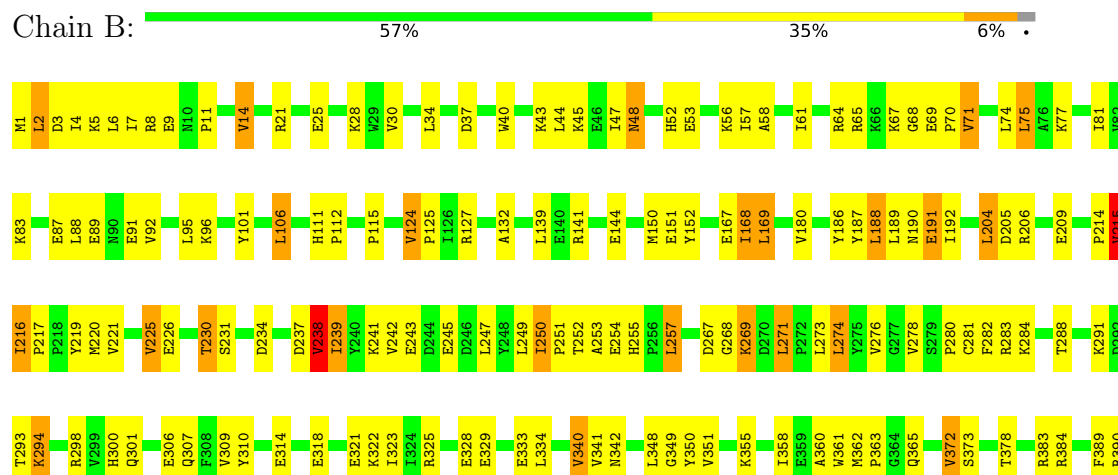
3 Residue-property plots

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: Seryl-tRNA synthetase



• Molecule 1: Seryl-tRNA synthetase



D391	R392	T393	D394	E395	V400	H401	S405	T406	A407	R412	V415	A416	E419	N420	D425	G426	T427	V428	R429	K432	W435	K436	Y437	K441	E442	I443	V444	P445	V446	E447	K448	LYS	GLU	ARG	CYS	CYS	ALA	THR
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	96.65Å 120.27Å 127.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.57 – 3.00 48.57 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.57-3.00) 99.9 (48.57-3.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.190 , 0.258 0.185 , 0.250	Depositor DCC
R_{free} test set	1537 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	84.1	Xtriage
Anisotropy	0.439	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 66.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7446	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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	0.53	0/3792	1.06	22/5120 (0.4%)
1	B	0.53	0/3792	1.08	15/5120 (0.3%)
All	All	0.53	0/7584	1.07	37/10240 (0.4%)

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	124	VAL	N-CA-C	12.58	121.60	107.89
1	A	395	GLU	N-CA-C	12.06	124.71	108.07
1	B	395	GLU	N-CA-C	10.91	124.72	110.43
1	B	407	ALA	N-CA-C	-10.75	97.40	112.13
1	A	407	ALA	N-CA-C	-10.73	97.74	112.12
1	B	238	VAL	N-CA-C	10.33	120.27	111.90
1	B	239	ILE	N-CA-C	9.96	122.04	108.89
1	A	351	VAL	N-CA-C	8.83	118.83	110.53
1	B	216	ILE	N-CA-C	-7.32	99.39	107.73
1	B	280	PRO	N-CA-C	-7.28	100.51	111.57
1	A	350	TYR	N-CA-C	7.24	119.80	111.11
1	B	250	ILE	N-CA-C	7.06	115.59	109.02
1	A	246	ASP	N-CA-C	-6.94	99.21	109.62
1	A	49	ARG	N-CA-C	-6.79	103.80	111.07
1	A	280	PRO	N-CA-C	-6.75	101.31	111.57
1	A	348	LEU	N-CA-C	6.52	118.47	111.36
1	B	237	ASP	N-CA-C	6.50	119.33	111.40
1	B	349	GLY	N-CA-C	-6.41	105.61	112.08
1	A	216	ILE	N-CA-C	-6.33	100.51	107.73
1	A	238	VAL	N-CA-C	6.27	122.37	109.34
1	B	215	VAL	N-CA-C	6.13	116.44	108.35
1	A	353	ALA	N-CA-C	-6.10	105.67	113.23
1	A	44	LEU	N-CA-C	-5.90	104.77	111.14
1	A	134	VAL	N-CA-C	5.89	116.36	108.11
1	A	415	VAL	N-CA-C	-5.87	104.61	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	345	THR	N-CA-C	5.67	117.46	111.28
1	B	350	TYR	N-CA-C	5.59	119.27	112.23
1	B	231	SER	N-CA-C	-5.41	102.47	110.48
1	A	352	ALA	N-CA-C	5.26	118.07	110.28
1	A	123	ASN	N-CA-C	-5.25	103.95	110.41
1	A	9	GLU	N-CA-C	5.23	119.66	113.28
1	A	239	ILE	N-CA-C	5.23	116.32	109.21
1	B	446	VAL	N-CA-C	-5.23	102.34	109.55
1	B	348	LEU	N-CA-C	5.19	116.79	111.03
1	A	409	ALA	N-CA-C	-5.18	98.12	107.75
1	A	244	ASP	N-CA-C	5.08	118.61	111.90
1	A	152	TYR	N-CA-C	5.04	115.69	108.74

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	3708	0	3750	165	0
1	B	3708	0	3750	154	0
2	A	13	0	0	1	0
2	B	17	0	0	0	0
All	All	7446	0	7500	305	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 20.

All (305) 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:288:THR:HG21	1:B:298:ARG:HD3	1.44	0.99
1:B:372:VAL:HB	1:B:406:THR:HB	1.55	0.89
1:A:127:ARG:HB3	1:A:340:VAL:HG22	1.55	0.87
1:A:269:LYS:HE2	1:A:269:LYS:HA	1.56	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:THR:HG21	1:B:234:ASP:OD2	1.77	0.85
1:B:318:GLU:O	1:B:322:LYS:HG3	1.79	0.82
1:B:358:ILE:HB	1:B:372:VAL:HG22	1.64	0.79
1:B:3:ASP:OD1	1:B:5:LYS:HE3	1.83	0.78
1:A:8:ARG:HD3	1:A:37:ASP:OD2	1.86	0.75
1:A:372:VAL:HB	1:A:406:THR:HB	1.69	0.74
1:A:446:VAL:O	1:A:447:GLU:HB2	1.85	0.74
1:B:43:LYS:HE2	1:B:91:GLU:OE2	1.88	0.74
1:B:52:HIS:NE2	1:B:56:LYS:HE3	2.02	0.74
1:A:1:MET:HE3	1:A:104:TRP:CD1	2.24	0.73
1:A:131:LYS:HE2	1:A:153:GLU:HB2	1.69	0.73
1:A:1:MET:H1	1:A:384:ARG:HH21	1.37	0.73
1:B:1:MET:HE2	1:B:383:ARG:HG2	1.70	0.73
1:A:105:ARG:HG2	1:A:105:ARG:HH11	1.53	0.72
1:A:220:MET:HE2	1:B:282:PHE:HD2	1.54	0.72
1:B:127:ARG:NH2	1:B:328:GLU:OE2	2.22	0.72
1:A:220:MET:HE2	1:B:282:PHE:CD2	2.26	0.71
1:B:58:ALA:O	1:B:61:ILE:HG22	1.91	0.71
1:A:392:ARG:HH21	1:A:393:THR:HG23	1.56	0.70
1:B:291:LYS:HE3	1:B:298:ARG:NH1	2.05	0.70
1:A:11:PRO:O	1:A:14:VAL:HG12	1.91	0.70
1:A:127:ARG:HB3	1:A:340:VAL:CG2	2.22	0.70
1:A:396:LYS:NZ	1:A:397:PRO:HD2	2.08	0.69
1:B:48:ASN:HD22	1:B:48:ASN:H	1.43	0.67
1:B:40:TRP:HE1	1:B:96:LYS:HE3	1.59	0.67
1:B:427:THR:HG22	1:B:445:PRO:HD3	1.75	0.67
1:B:2:LEU:HD22	1:B:106:LEU:HB3	1.76	0.66
1:A:40:TRP:HD1	1:A:92:VAL:HG13	1.60	0.66
1:B:71:VAL:O	1:B:75:LEU:HB2	1.95	0.66
1:B:378:THR:O	1:B:401:HIS:HA	1.95	0.66
1:B:65:ARG:O	1:B:65:ARG:HD3	1.96	0.65
1:A:394:ASP:OD2	1:A:395:GLU:HG2	1.96	0.65
1:B:269:LYS:H	1:B:269:LYS:HD2	1.62	0.65
1:A:371:VAL:HG12	1:A:372:VAL:HG13	1.77	0.65
1:B:360:ALA:HB3	1:B:362:MET:HE2	1.78	0.65
1:A:61:ILE:HG23	1:A:71:VAL:HG11	1.78	0.65
1:A:402:THR:C	1:A:403:LEU:HD12	2.22	0.65
1:A:447:GLU:O	1:A:448:LYS:HB2	1.96	0.65
1:A:178:ALA:HA	1:A:182:GLY:O	1.97	0.64
1:A:249:LEU:HD21	1:B:249:LEU:HD11	1.79	0.64
1:B:253:ALA:O	1:B:257:LEU:HB2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:ARG:HD3	1:B:65:ARG:C	2.22	0.64
1:A:49:ARG:HG3	1:A:49:ARG:HH11	1.63	0.64
1:B:205:ASP:O	1:B:209:GLU:HG3	1.97	0.64
1:B:242:VAL:HG13	1:B:245:GLU:HB2	1.79	0.64
1:B:186:TYR:CD2	1:B:188:LEU:HD13	2.32	0.63
1:A:69:GLU:N	1:A:70:PRO:HD3	2.14	0.63
1:B:273:LEU:HB2	1:B:310:TYR:HB2	1.81	0.62
1:A:59:VAL:HG23	1:A:63:LYS:HE2	1.81	0.62
1:A:260:MET:HE3	1:B:187:TYR:CE2	2.35	0.62
1:A:147:GLN:HE21	1:A:149:LYS:HD2	1.65	0.62
1:B:61:ILE:HG13	1:B:71:VAL:HG11	1.81	0.62
1:B:21:ARG:HG2	1:B:21:ARG:HH21	1.64	0.62
1:A:392:ARG:HE	1:A:393:THR:H	1.45	0.61
1:B:1:MET:H1	1:B:384:ARG:HH21	1.47	0.61
1:B:48:ASN:HD22	1:B:48:ASN:N	1.98	0.61
1:B:1:MET:O	1:B:383:ARG:HD2	2.00	0.61
1:B:425:ASP:CG	1:B:427:THR:HG23	2.25	0.61
1:B:1:MET:HE2	1:B:383:ARG:CG	2.31	0.61
1:A:378:THR:O	1:A:401:HIS:HA	2.01	0.60
1:A:78:SER:O	1:A:82:VAL:HG23	2.01	0.60
1:B:53:GLU:O	1:B:57:ILE:HG12	2.00	0.60
1:B:291:LYS:HE3	1:B:298:ARG:HH12	1.66	0.60
1:A:195:LEU:O	1:A:198:ALA:HB3	2.01	0.60
1:B:276:VAL:HG13	1:B:276:VAL:O	1.99	0.60
1:B:169:LEU:HG	1:B:443:ILE:HG22	1.82	0.59
1:B:21:ARG:HG2	1:B:21:ARG:NH2	2.18	0.59
1:A:251:PRO:HG2	1:A:252:THR:HG22	1.84	0.59
1:B:191:GLU:HG3	1:B:443:ILE:HG23	1.84	0.59
1:B:251:PRO:HG2	1:B:252:THR:HG22	1.84	0.59
1:B:69:GLU:N	1:B:70:PRO:HD3	2.16	0.58
1:A:190:ASN:HA	1:B:214:PRO:HG2	1.83	0.58
1:A:13:LEU:C	1:A:13:LEU:HD13	2.27	0.58
1:A:24:LEU:O	1:A:27:VAL:HG12	2.03	0.58
1:B:87:GLU:O	1:B:91:GLU:HG3	2.03	0.58
1:B:127:ARG:HH21	1:B:328:GLU:CD	2.12	0.58
1:A:105:ARG:HH11	1:A:105:ARG:CG	2.17	0.57
1:B:43:LYS:O	1:B:47:ILE:HG13	2.03	0.57
1:A:222:ARG:HG3	1:A:246:ASP:OD1	2.05	0.57
1:B:436:LYS:HE2	1:B:437:TYR:CE1	2.40	0.57
1:A:37:ASP:O	1:A:41:ARG:HG2	2.04	0.57
1:A:145:GLN:HG3	2:A:457:HOH:O	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:VAL:HG22	1:B:216:ILE:HG13	1.88	0.56
1:B:1:MET:HE2	1:B:383:ARG:CD	2.36	0.56
1:B:220:MET:HE2	1:B:247:LEU:HD13	1.86	0.56
1:B:115:PRO:HD3	1:B:342:ASN:ND2	2.21	0.56
1:A:392:ARG:HB3	1:A:394:ASP:OD1	2.06	0.55
1:B:7:ILE:N	1:B:7:ILE:HD12	2.21	0.55
1:A:14:VAL:HG13	1:A:15:LYS:N	2.20	0.55
1:A:214:PRO:HG2	1:B:190:ASN:HA	1.89	0.55
1:A:40:TRP:CD1	1:A:92:VAL:HG13	2.42	0.54
1:A:219:TYR:CE2	1:A:280:PRO:HD2	2.42	0.54
1:A:241:LYS:HD2	1:A:248:TYR:CE2	2.42	0.54
1:B:61:ILE:HG13	1:B:71:VAL:CG1	2.38	0.54
1:B:67:LYS:HG2	1:B:68:GLY:H	1.71	0.54
1:B:412:ARG:O	1:B:415:VAL:HG22	2.07	0.54
1:B:226:GLU:OE1	1:B:255:HIS:ND1	2.40	0.54
1:B:69:GLU:C	1:B:71:VAL:H	2.15	0.54
1:B:151:GLU:O	1:B:152:TYR:HB3	2.07	0.54
1:B:61:ILE:CD1	1:B:75:LEU:HD23	2.38	0.54
1:B:83:LYS:O	1:B:87:GLU:HG3	2.08	0.53
1:B:141:ARG:O	1:B:144:GLU:HB3	2.09	0.53
1:A:35:LYS:O	1:A:39:GLU:HG3	2.09	0.53
1:A:396:LYS:HZ2	1:A:397:PRO:HD2	1.73	0.53
1:B:242:VAL:CG1	1:B:247:LEU:HB2	2.39	0.53
1:A:376:ASN:HA	1:A:403:LEU:HG	1.91	0.53
1:B:219:TYR:O	1:B:250:ILE:HG23	2.10	0.52
1:B:5:LYS:O	1:B:9:GLU:HG3	2.09	0.52
1:B:363:PRO:HG2	1:B:420:ASN:HA	1.91	0.52
1:A:165:LEU:HD23	1:A:168:ILE:HD11	1.92	0.52
1:B:204:LEU:HD21	1:B:278:VAL:HG21	1.92	0.52
1:A:205:ASP:O	1:A:209:GLU:HG3	2.10	0.51
1:A:316:SER:HB2	1:A:376:ASN:HD21	1.75	0.51
1:A:129:TRP:CH2	1:A:332:GLN:HA	2.45	0.51
1:A:321:GLU:O	1:A:325:ARG:HG2	2.10	0.51
1:A:396:LYS:NZ	1:A:396:LYS:HA	2.25	0.51
1:A:124:VAL:O	1:A:126:ILE:HG23	2.10	0.51
1:A:304:LYS:HD3	1:A:306:GLU:OE1	2.10	0.51
1:A:14:VAL:CG1	1:A:15:LYS:N	2.73	0.51
1:B:252:THR:C	1:B:254:GLU:H	2.19	0.51
1:B:435:TRP:CE2	1:B:441:LYS:HG2	2.45	0.51
1:A:339:ARG:O	1:A:339:ARG:HG3	2.11	0.51
1:A:362:MET:HB3	1:A:419:GLU:OE1	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:GLU:HA	1:A:63:LYS:HE3	1.93	0.51
1:B:74:LEU:O	1:B:74:LEU:HD23	2.10	0.51
1:A:392:ARG:HE	1:A:393:THR:N	2.10	0.50
1:B:425:ASP:OD2	1:B:427:THR:HG23	2.11	0.50
1:A:26:LYS:HE2	1:A:29:TRP:CH2	2.47	0.50
1:A:169:LEU:HG	1:A:443:ILE:HG22	1.94	0.50
1:A:7:ILE:HG22	1:A:34:LEU:HD21	1.93	0.50
1:B:69:GLU:HG2	1:B:71:VAL:HG22	1.93	0.50
1:B:390:ARG:HD3	1:B:392:ARG:O	2.11	0.50
1:A:180:VAL:HG12	1:A:181:SER:OG	2.11	0.50
1:B:4:ILE:HD11	1:B:37:ASP:OD1	2.11	0.50
1:B:14:VAL:HG22	1:B:30:VAL:HG21	1.93	0.50
1:B:186:TYR:HD2	1:B:188:LEU:HD13	1.77	0.49
1:B:416:ALA:O	1:B:420:ASN:HB2	2.11	0.49
1:B:25:GLU:OE2	1:B:28:LYS:HD2	2.13	0.49
1:A:189:LEU:HD23	1:B:215:VAL:HB	1.94	0.49
1:A:240:TYR:HA	1:A:284:LYS:HE3	1.95	0.48
1:A:147:GLN:C	1:A:149:LYS:H	2.20	0.48
1:B:281:CYS:O	1:B:301:GLN:HA	2.13	0.48
1:B:68:GLY:C	1:B:70:PRO:HD3	2.38	0.48
1:B:238:VAL:HG22	1:B:239:ILE:HG13	1.94	0.48
1:B:220:MET:HE2	1:B:247:LEU:CD1	2.44	0.48
1:A:219:TYR:CG	1:B:301:GLN:NE2	2.82	0.48
1:A:392:ARG:HA	1:A:392:ARG:NE	2.27	0.48
1:A:423:GLU:OE2	1:A:429:ARG:HD2	2.14	0.48
1:B:321:GLU:O	1:B:325:ARG:HG3	2.14	0.48
1:A:8:ARG:HH22	1:A:40:TRP:HZ3	1.62	0.48
1:A:223:ARG:HB2	1:A:248:TYR:CE1	2.49	0.48
1:A:276:VAL:O	1:A:276:VAL:HG13	2.14	0.48
1:A:77:LYS:O	1:A:81:ILE:HG13	2.14	0.47
1:A:173:ASP:OD2	1:A:176:ARG:HD2	2.14	0.47
1:B:64:ARG:HB3	1:B:69:GLU:HA	1.96	0.47
1:A:370:GLU:HG2	1:A:371:VAL:N	2.28	0.47
1:A:273:LEU:HB2	1:A:310:TYR:HB2	1.95	0.47
1:B:169:LEU:HG	1:B:443:ILE:CG2	2.44	0.47
1:A:68:GLY:C	1:A:70:PRO:HD3	2.39	0.47
1:A:219:TYR:CZ	1:A:280:PRO:HD2	2.49	0.47
1:A:105:ARG:CG	1:A:105:ARG:NH1	2.74	0.47
1:A:207:LEU:N	1:A:207:LEU:HD22	2.28	0.47
1:A:208:ILE:HG12	1:A:214:PRO:HD3	1.96	0.47
1:A:303:HIS:HB2	1:A:410:THR:OG1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:LEU:HD12	1:A:106:LEU:HB3	1.96	0.47
1:B:132:ALA:HB2	1:B:150:MET:HE2	1.97	0.47
1:B:111:HIS:CD2	1:B:112:PRO:HD2	2.49	0.47
1:A:222:ARG:HG3	1:A:246:ASP:CG	2.40	0.46
1:A:307:GLN:OE1	1:A:323:ILE:HG22	2.15	0.46
1:B:75:LEU:HD13	1:B:75:LEU:O	2.15	0.46
1:B:239:ILE:O	1:B:284:LYS:HE3	2.15	0.46
1:B:427:THR:HG22	1:B:445:PRO:CD	2.42	0.46
1:A:343:ILE:HD11	1:A:357:ASP:CG	2.41	0.46
1:A:435:TRP:CH2	1:A:441:LYS:HD3	2.51	0.46
1:A:64:ARG:HB3	1:A:69:GLU:HA	1.98	0.46
1:A:59:VAL:O	1:A:63:LYS:HD3	2.15	0.46
1:A:108:ASN:HD22	1:A:380:TRP:HB2	1.80	0.46
1:A:358:ILE:HB	1:A:372:VAL:HG22	1.97	0.46
1:A:395:GLU:HB2	1:A:396:LYS:H	1.51	0.46
1:B:288:THR:HG21	1:B:298:ARG:CD	2.29	0.46
1:A:39:GLU:HB2	1:A:95:LEU:HD21	1.97	0.46
1:A:120:GLU:H	1:A:120:GLU:CD	2.24	0.46
1:A:51:ARG:HG2	1:A:54:ARG:NH2	2.31	0.45
1:A:69:GLU:C	1:A:71:VAL:H	2.25	0.45
1:A:333:GLU:O	1:A:433:VAL:HG21	2.17	0.45
1:A:343:ILE:HD11	1:A:357:ASP:OD2	2.16	0.45
1:B:250:ILE:O	1:B:250:ILE:HG13	2.14	0.45
1:B:267:ASP:OD2	1:B:269:LYS:HB2	2.16	0.45
1:A:260:MET:HE3	1:B:187:TYR:CD2	2.51	0.45
1:B:329:GLU:O	1:B:333:GLU:HG3	2.17	0.45
1:A:62:GLY:O	1:A:65:ARG:HB3	2.17	0.45
1:A:288:THR:HG23	1:A:288:THR:O	2.16	0.45
1:B:191:GLU:HG3	1:B:443:ILE:CG2	2.46	0.45
1:B:325:ARG:HG2	1:B:325:ARG:HH11	1.82	0.45
1:B:101:TYR:CD2	1:B:101:TYR:C	2.94	0.45
1:A:207:LEU:N	1:A:207:LEU:CD2	2.79	0.45
1:A:396:LYS:HZ2	1:A:396:LYS:HA	1.81	0.45
1:B:306:GLU:HG3	1:B:307:GLN:N	2.31	0.45
1:B:314:GLU:H	1:B:314:GLU:CD	2.24	0.45
1:B:429:ARG:NH2	1:B:442:GLU:OE1	2.49	0.45
1:A:269:LYS:HA	1:A:269:LYS:CE	2.37	0.45
1:A:368:PHE:O	1:A:369:ARG:HD2	2.17	0.45
1:B:355:LYS:HE3	1:B:373:SER:OG	2.17	0.45
1:A:101:TYR:O	1:A:105:ARG:HG3	2.17	0.44
1:B:40:TRP:HE1	1:B:96:LYS:CE	2.28	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:ARG:HH21	1:A:21:ARG:HG2	1.82	0.44
1:A:124:VAL:HA	1:A:125:PRO:HD3	1.81	0.44
1:A:253:ALA:O	1:A:257:LEU:HB2	2.16	0.44
1:A:432:LYS:HG2	1:A:435:TRP:CH2	2.53	0.44
1:A:94:GLU:OE1	1:A:94:GLU:HA	2.18	0.44
1:A:447:GLU:O	1:A:448:LYS:CB	2.63	0.44
1:B:61:ILE:HB	1:B:74:LEU:CD2	2.48	0.44
1:B:92:VAL:CG1	1:B:96:LYS:HE3	2.47	0.44
1:A:67:LYS:HG2	1:A:68:GLY:H	1.81	0.44
1:A:257:LEU:HD12	1:A:257:LEU:HA	1.91	0.44
1:B:252:THR:C	1:B:254:GLU:N	2.72	0.44
1:B:221:VAL:HG21	1:B:225:VAL:HG22	1.99	0.44
1:A:333:GLU:HB3	1:A:433:VAL:HG21	1.99	0.44
1:B:21:ARG:HH21	1:B:21:ARG:CG	2.30	0.44
1:B:274:LEU:HD12	1:B:309:VAL:HG22	2.00	0.44
1:A:147:GLN:O	1:A:149:LYS:HG3	2.17	0.44
1:A:108:ASN:ND2	1:A:380:TRP:HB2	2.33	0.44
1:B:1:MET:HE2	1:B:383:ARG:HD3	2.00	0.44
1:B:242:VAL:HG11	1:B:247:LEU:HB2	1.99	0.43
1:A:105:ARG:HG2	1:A:105:ARG:NH1	2.28	0.43
1:B:52:HIS:CD2	1:B:56:LYS:HE3	2.53	0.43
1:B:127:ARG:CZ	1:B:325:ARG:HH12	2.32	0.43
1:A:126:ILE:CG1	1:A:340:VAL:HG23	2.49	0.43
1:A:184:ARG:HG2	1:A:184:ARG:HH21	1.83	0.43
1:A:374:ALA:HA	1:A:405:SER:HB2	2.00	0.43
1:B:323:ILE:HD12	1:B:405:SER:HB2	2.00	0.43
1:A:343:ILE:HD12	1:A:355:LYS:HG2	2.01	0.43
1:B:269:LYS:HD2	1:B:269:LYS:N	2.32	0.43
1:A:2:LEU:HD23	1:A:2:LEU:HA	1.72	0.43
1:A:158:LYS:HA	1:A:159:PRO:HD3	1.89	0.43
1:B:77:LYS:O	1:B:81:ILE:HG13	2.18	0.43
1:B:115:PRO:HD3	1:B:342:ASN:HD21	1.82	0.43
1:B:168:ILE:O	1:B:446:VAL:HG22	2.19	0.43
1:B:242:VAL:HG12	1:B:247:LEU:O	2.19	0.43
1:A:204:LEU:HD12	1:A:204:LEU:HA	1.71	0.42
1:A:208:ILE:HD11	1:A:214:PRO:HG3	2.00	0.42
1:A:306:GLU:HG3	1:A:307:GLN:N	2.34	0.42
1:A:429:ARG:NH1	1:A:442:GLU:OE1	2.50	0.42
1:B:191:GLU:HB2	1:B:443:ILE:CD1	2.49	0.42
1:B:267:ASP:O	1:B:268:GLY:C	2.62	0.42
1:B:282:PHE:HA	1:B:300:HIS:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:THR:OG1	1:A:379:ASP:N	2.52	0.42
1:B:188:LEU:HG	1:B:192:ILE:HG22	2.01	0.42
1:B:191:GLU:CD	1:B:191:GLU:H	2.27	0.42
1:A:24:LEU:C	1:A:26:LYS:N	2.78	0.42
1:A:50:LEU:HD22	1:A:81:ILE:HG23	2.02	0.42
1:A:249:LEU:HD11	1:B:249:LEU:HD21	2.01	0.42
1:A:190:ASN:O	1:A:191:GLU:C	2.63	0.42
1:A:206:ARG:HH21	1:A:333:GLU:CD	2.28	0.42
1:A:432:LYS:HA	1:A:435:TRP:CE2	2.55	0.42
1:B:88:LEU:O	1:B:89:GLU:C	2.61	0.42
1:B:124:VAL:HA	1:B:125:PRO:HD3	1.91	0.42
1:B:429:ARG:HG2	1:B:429:ARG:HH21	1.84	0.42
1:B:132:ALA:HB1	1:B:361:TRP:CD1	2.55	0.42
1:A:394:ASP:CG	1:A:395:GLU:N	2.77	0.42
1:A:206:ARG:NH2	1:A:333:GLU:OE1	2.51	0.41
1:B:74:LEU:HD23	1:B:74:LEU:C	2.45	0.41
1:B:429:ARG:NH2	1:B:429:ARG:HG2	2.34	0.41
1:A:241:LYS:NZ	1:B:243:GLU:OE2	2.51	0.41
1:A:269:LYS:HE2	1:A:269:LYS:CA	2.40	0.41
1:B:3:ASP:CG	1:B:5:LYS:HE3	2.43	0.41
1:A:43:LYS:O	1:A:47:ILE:HG13	2.19	0.41
1:B:389:PHE:CD1	1:B:400:VAL:HG12	2.54	0.41
1:B:61:ILE:HD12	1:B:75:LEU:HD23	2.01	0.41
1:B:365:GLN:HG3	1:B:419:GLU:OE1	2.21	0.41
1:A:354:LYS:HE2	1:A:356:TYR:CZ	2.55	0.41
1:B:11:PRO:HB3	1:B:34:LEU:HD11	2.01	0.41
1:A:2:LEU:HD12	1:A:106:LEU:CB	2.51	0.41
1:A:73:GLU:O	1:A:76:ALA:HB3	2.20	0.41
1:B:390:ARG:CD	1:B:393:THR:HA	2.51	0.41
1:A:243:GLU:OE1	1:B:241:LYS:HD3	2.20	0.41
1:A:186:TYR:CD2	1:A:188:LEU:HD13	2.56	0.41
1:A:320:HIS:HA	1:A:403:LEU:HD23	2.01	0.41
1:A:335:GLU:HB2	1:A:421:HIS:CE1	2.55	0.41
1:B:328:GLU:O	1:B:329:GLU:C	2.63	0.41
1:A:358:ILE:CG1	1:A:372:VAL:HG22	2.51	0.41
1:B:271:LEU:HD12	1:B:271:LEU:HA	1.88	0.41
1:A:88:LEU:HD23	1:A:88:LEU:HA	1.86	0.41
1:A:242:VAL:CG2	1:A:245:GLU:HB2	2.50	0.41
1:A:21:ARG:HG2	1:A:21:ARG:NH2	2.36	0.40
1:A:26:LYS:O	1:A:29:TRP:HB2	2.20	0.40
1:A:281:CYS:O	1:A:301:GLN:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:PHE:CD1	1:A:412:ARG:HG2	2.56	0.40
1:A:369:ARG:HG3	1:A:369:ARG:HH21	1.86	0.40
1:B:323:ILE:HD12	1:B:405:SER:CB	2.52	0.40
1:A:95:LEU:O	1:A:99:ILE:HG13	2.21	0.40
1:A:324:ILE:O	1:A:328:GLU:HG3	2.22	0.40
1:A:371:VAL:CG1	1:A:372:VAL:HG13	2.46	0.40
1:B:3:ASP:HB2	1:B:383:ARG:CZ	2.51	0.40
1:B:8:ARG:NH2	1:B:37:ASP:OD1	2.54	0.40
1:B:127:ARG:HB2	1:B:340:VAL:HG13	2.04	0.40
1:A:215:VAL:HB	1:B:189:LEU:HD23	2.03	0.40
1:B:8:ARG:HA	1:B:34:LEU:HD21	2.03	0.40
1:A:8:ARG:NH2	1:A:37:ASP:OD1	2.54	0.40
1:A:65:ARG:HG3	1:A:65:ARG:HH11	1.86	0.40
1:B:2:LEU:HD12	1:B:2:LEU:HA	1.87	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	446/455 (98%)	409 (92%)	31 (7%)	6 (1%)	9	38
1	B	446/455 (98%)	414 (93%)	30 (7%)	2 (0%)	30	65
All	All	892/910 (98%)	823 (92%)	61 (7%)	8 (1%)	14	48

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	294	LYS
1	A	190	ASN
1	B	294	LYS
1	A	447	GLU

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Mol	Chain	Res	Type
1	A	25	GLU
1	A	396	LYS
1	B	71	VAL
1	A	71	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	399/405 (98%)	362 (91%)	37 (9%)	8	32
1	B	399/405 (98%)	358 (90%)	41 (10%)	7	28
All	All	798/810 (98%)	720 (90%)	78 (10%)	7	30

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	6	LEU
1	A	13	LEU
1	A	17	ASP
1	A	44	LEU
1	A	49	ARG
1	A	54	ARG
1	A	63	LYS
1	A	67	LYS
1	A	82	VAL
1	A	119	ASP
1	A	139	LEU
1	A	144	GLU
1	A	146	SER
1	A	167	GLU
1	A	188	LEU
1	A	191	GLU
1	A	204	LEU
1	A	215	VAL

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Mol	Chain	Res	Type
1	A	217	PRO
1	A	222	ARG
1	A	225	VAL
1	A	238	VAL
1	A	242	VAL
1	A	252	THR
1	A	257	LEU
1	A	269	LYS
1	A	278	VAL
1	A	306	GLU
1	A	312	ARG
1	A	334	LEU
1	A	341	VAL
1	A	371	VAL
1	A	372	VAL
1	A	396	LYS
1	A	429	ARG
1	A	444	VAL
1	B	2	LEU
1	B	6	LEU
1	B	14	VAL
1	B	44	LEU
1	B	45	LYS
1	B	48	ASN
1	B	75	LEU
1	B	95	LEU
1	B	106	LEU
1	B	139	LEU
1	B	167	GLU
1	B	168	ILE
1	B	169	LEU
1	B	180	VAL
1	B	188	LEU
1	B	191	GLU
1	B	204	LEU
1	B	206	ARG
1	B	215	VAL
1	B	217	PRO
1	B	225	VAL
1	B	230	THR
1	B	238	VAL
1	B	257	LEU

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Mol	Chain	Res	Type
1	B	269	LYS
1	B	271	LEU
1	B	274	LEU
1	B	283	ARG
1	B	293	THR
1	B	294	LYS
1	B	334	LEU
1	B	340	VAL
1	B	341	VAL
1	B	351	VAL
1	B	372	VAL
1	B	392	ARG
1	B	393	THR
1	B	394	ASP
1	B	427	THR
1	B	432	LYS
1	B	448	LYS

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	55	ASN
1	A	147	GLN
1	A	263	ASN
1	A	386	ASN
1	B	16	ASN
1	B	48	ASN
1	B	138	HIS
1	B	263	ASN
1	B	342	ASN
1	B	386	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	448/455 (98%)	-0.67	0 100 100	39, 70, 118, 163	0
1	B	448/455 (98%)	-0.73	0 100 100	36, 64, 126, 175	0
All	All	896/910 (98%)	-0.70	0 100 100	36, 68, 124, 175	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 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.