W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 12:47 am GMT

PDB ID	:	4ZP4
Title	:	Crystal Structure of the Heterodimeric HIF-2a:ARNT Complex
Authors	:	Wu, D.; Potluri, N.; Lu, J.; Kim, Y.; Rastinejad, F.
Deposited on	:	2015-05-07
Resolution	:	2.35 Å(reported)

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 2.35 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.
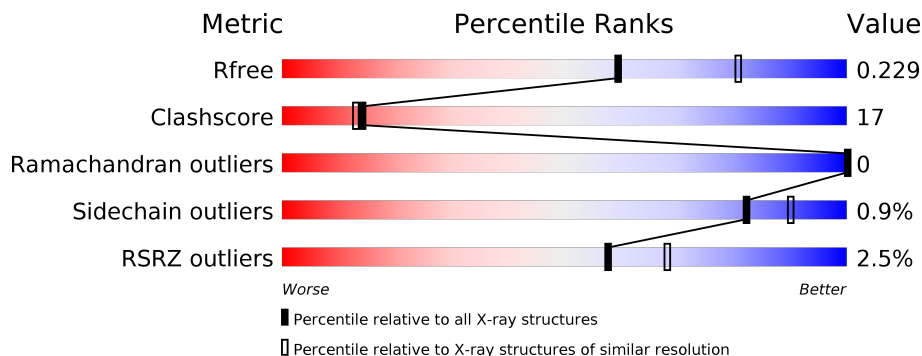
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1522 (2.38-2.34)
Clashscore	112137	1626 (2.38-2.34)
Ramachandran outliers	110173	1605 (2.38-2.34)
Sidechain outliers	110143	1606 (2.38-2.34)
RSRZ outliers	101464	1528 (2.38-2.34)

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 >=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 <=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	384	2% / 40% 28% • 32%
1	C	384	% / 40% 27% • 33%
2	B	360	2% / 53% 28% 18%
2	D	360	3% / 56% 24% 20%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 9063 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 Aryl hydrocarbon receptor nuclear translocator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total 2124	C 1348	N 374	O 386	S 16	0	0	0
1	C	258	Total 2101	C 1332	N 371	O 382	S 16	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	81	MET	-	initiating methionine	UNP P53762
C	81	MET	-	initiating methionine	UNP P53762

- Molecule 2 is a protein called Endothelial PAS domain-containing protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	295	Total 2374	C 1498	N 408	O 444	S 24	0	0	0
2	D	288	Total 2325	C 1474	N 394	O 435	S 22	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	2	MET	-	initiating methionine	UNP P97481
D	2	MET	-	initiating methionine	UNP P97481

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	28	Total 28	O 28	0	0
3	B	35	Total 35	O 35	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	32	Total 32	O 32	0	0
3	D	44	Total 44	O 44	0	0

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: Aryl hydrocarbon receptor nuclear translocator

- Molecule 1: Aryl hydrocarbon receptor nuclear translocator

F375 V376 D377 H378 R379 C380 V381 A382 T383 V384 G385 Y386 Q387 P388 Q389 E390 L391 L392 V397 E398 F399 C400 H401 P402 E403 D404 D410 S411 F412 Q413 Q414 V415 V416 K417 L418 K419 G420 Q421 M426 F427 R428 F429 R430 T433 R434 E435 W436 M439 R440 F446 Q447 S451

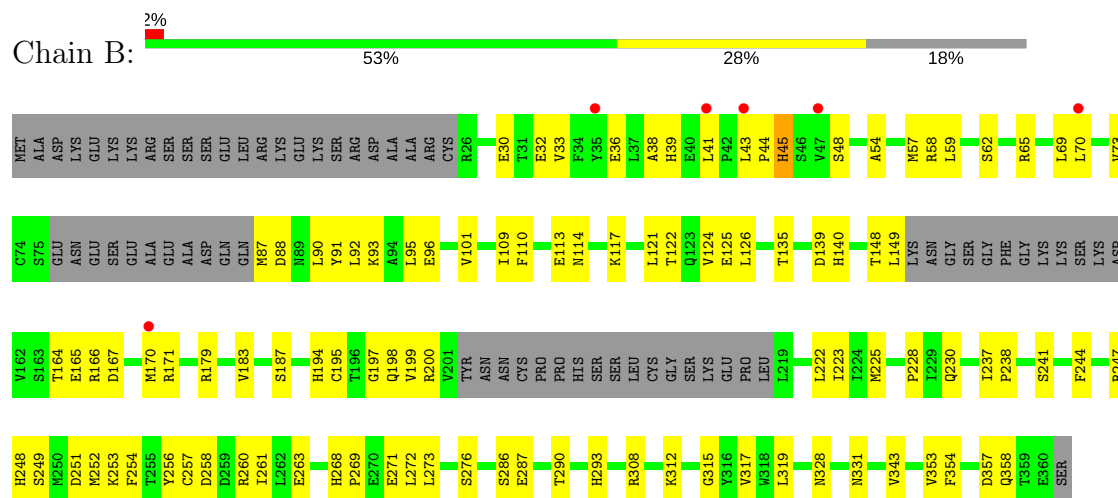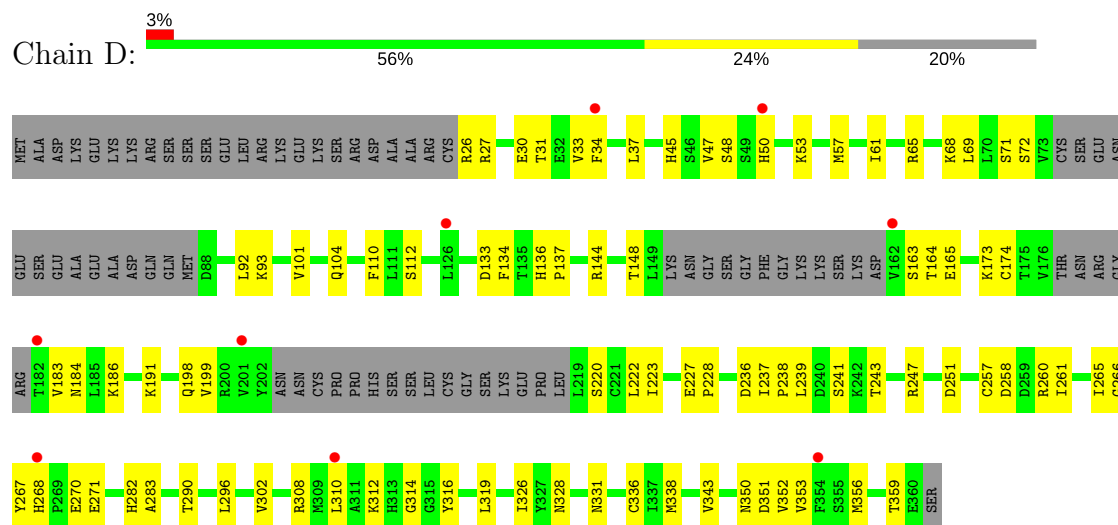Y456 I457 I458 C459 V464

• Molecule 2: Endothelial PAS domain-containing protein 1

Chain B:

MET ALA ASP LYS GLU LYS LYS ARG SER SER SER GLU GLU LEU ARG LYS GLU LYS SER GLU SER ARG ASP ALA ALA ARG CYS R26 E30 T31 E32 V33 F34 Y35 E36 L37 A38 H39 E40 L41 P42 L43 P44 H45 S46 V47 S48 A54 M57 R58 L59 S62 R65 L69 L70 V73

C74 S75 GLU ASN GLU SER GLU ALA GLU ALA ASP GLN GLN GLN M87 D88 N89 L90 Y91 L92 K93 A94 L95 E96 V101 I109 F110 E113 N114 K117 L121 T122 Q123 V124 E125 L126 T135 D139 H140 T148 L149 LYS ASN GLY SER GLY PHE GLY LYS LYS SER LYS ASP

V162 S163 T164 E165 R166 D167 M170 R171 R179 V183 S187 H194 C195 T196 G197 Q198 V199 R200 V201 TYR ASN ASN CYS PRO PRO HIS SER SER LEU CYS GLY LYS SER GLU PRO LEU L219 L222 I223 I224 M225 P228 I229 Q230 I237 P238 S241 F244 R247

H248 S249 M250 D251 M252 K253 F254 T255 Y256 C257 D258 D259 R260 I261 L262 E263 H268 P269 E270 E271 L272 L273 S276 S286 E287 T290 H293 R308 K312 G315 Y316 V317 W318 L319 N328 N331 V343 V353 F354 D357 Q358 T359 E360 SER

• Molecule 2: Endothelial PAS domain-containing protein 1

Chain D:

MET ALA ASP LYS GLU LYS LYS ARG SER SER SER GLU LEU ARG LYS GLU LYS SER GLU SER ARG ASP ALA ALA ARG CYS R26 R27 E30 T31 E32 V33 F34 L37 H45 S46 V47 S48 S49 H50 K53 M57 I61 R65 K68 L69 L70 S71 S72 V73 CYS SER GLU ASN

GLU SER GLU ALA GLU ALA ASP GLN GLN MET D88 L92 K93 V101 Q104 F110 L111 S112 L126 D133 F134 T135 H136 P137 R144 T148 L149 LYS ASN GLY SER GLY PHE GLY LYS LYS SER LYS ASP V162 S163 T164 E165 K173 C174 T175 V176 THR ASN ARG GLY

ARG T182 V183 N184 L185 K186 K191 Q198 V199 R200 V201 Y202 ASN ASN CYS PRO PRO HIS SER SER LEU CYS GLY SER LYS GLU PRO LEU L219 S220 C221 L222 I223 E227 P228 D236 I237 P238 L239 D240 S241 K242 T243 R247 D251 C257 D258 D259 R260 I261 I265 G266

Y267 H268 P269 E270 E271 H282 A283 T290 L296 V302 R308 M309 L310 A311 K312 H313 G314 G315 Y316 L319 I326 Y327 N328 N331 C336 I337 M338 V343 N350 D351 V352 V353 F354 S355 M356 T359 E360 SER

4　Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	49.01Å　　76.46Å　　98.82Å 90.06°　　90.19°　　73.13°	Depositor
Resolution (Å)	49.41　–　2.35 49.41　–　2.36	Depositor EDS
% Data completeness (in resolution range)	98.2 (49.41-2.35) 97.4 (49.41-2.36)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.62 (at 2.37Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.200　,　0.232 0.207　,　0.229	Depositor DCC
R_{free} test set	2827 reflections (5.34%)	DCC
Wilson B-factor (Å^2)	55.0	Xtriage
Anisotropy	0.245	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 70.2	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.019 for h,h-k,-l 0.448 for -h,-k,l 0.018 for -h,-h+k,-l	Xtriage
Reported twinning fraction	0.470 for -h,-k,l	Depositor
Outliers	0 of 55771 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9063	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.53% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.54	0/2166	0.69	0/2920
1	C	0.54	0/2142	0.68	0/2886
2	B	0.55	0/2421	0.68	0/3265
2	D	0.57	0/2372	0.71	0/3200
All	All	0.55	0/9101	0.69	0/12271

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 ⓘ

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	2124	0	2118	94	0
1	C	2101	0	2090	91	0
2	B	2374	0	2341	81	0
2	D	2325	0	2288	77	0
3	A	28	0	0	1	0
3	B	35	0	0	0	0
3	C	32	0	0	0	0
3	D	44	0	0	0	0
All	All	9063	0	8837	309	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 17.

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PROTEIN DATA BANK

All (309) 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:A:163:GLU:HG2	2:B:70:LEU:HD12	1.29	1.12
1:A:160:THR:HB	1:A:163:GLU:HB2	1.45	0.96
1:A:164:LEU:O	1:A:164:LEU:HD12	1.79	0.82
2:D:266:GLY:HA3	2:D:312:LYS:HG2	1.63	0.80
2:B:54:ALA:O	2:B:58:ARG:HG3	1.88	0.73
2:D:241:SER:HA	2:D:260:ARG:HH11	1.55	0.70
1:A:189:VAL:HG11	1:A:204:TRP:HB3	1.74	0.70
1:C:428:ARG:HB3	1:C:436:TRP:HB3	1.74	0.70
2:D:239:LEU:HD13	2:D:243:THR:HG21	1.73	0.70
1:C:132:LEU:O	1:C:136:VAL:HG23	1.92	0.69
1:A:207:SER:OG	1:A:208:THR:N	2.25	0.68
1:A:181:CYS:HB2	1:A:335:PHE:HB2	1.75	0.68
1:C:387:GLN:HB3	1:C:389:GLN:OE1	1.94	0.68
1:A:377:ASP:OD2	1:A:379:ARG:NH2	2.23	0.67
1:A:440:ARG:NH2	1:A:462:THR:OG1	2.27	0.67
1:C:172:ALA:HB1	1:C:342:ARG:HD3	1.77	0.67
1:A:390:GLU:OE2	1:A:432:LYS:NZ	2.21	0.65
1:C:386:TYR:OH	1:C:430:ARG:NH1	2.28	0.65
1:A:315:TRP:HB3	1:A:336:CYS:HB2	1.78	0.64
2:B:269:PRO:O	2:B:273:LEU:HG	1.97	0.64
2:D:164:THR:OG1	2:D:198:GLN:NE2	2.31	0.64
2:D:101:VAL:HB	2:D:110:PHE:HB3	1.79	0.63
1:C:110:THR:O	1:C:113:SER:OG	2.14	0.63
1:A:105:MET:O	1:A:109:ILE:HG12	1.97	0.63
1:A:313:LYS:HG3	1:A:313:LYS:O	1.99	0.62
1:C:260:ARG:NH2	2:D:93:LYS:O	2.31	0.62
1:C:399:PHE:O	1:C:430:ARG:N	2.30	0.62
1:C:433:THR:O	1:C:434:ARG:HB2	2.00	0.62
1:A:175:PHE:HB2	1:A:192:SER:HB2	1.81	0.62
2:D:174:CYS:SG	2:D:191:LYS:HE2	2.40	0.62
2:B:135:THR:O	2:B:140:HIS:NE2	2.33	0.61
2:D:165:GLU:N	2:D:165:GLU:OE1	2.32	0.61
2:B:179:ARG:HG2	2:B:179:ARG:O	2.01	0.61
2:B:268:HIS:HB2	2:B:271:GLU:HG3	1.83	0.61
1:C:381:VAL:HG22	1:C:387:GLN:HA	1.83	0.60
1:C:366:ARG:HB2	1:C:375:PHE:HB3	1.83	0.60
1:A:164:LEU:C	1:A:164:LEU:HD12	2.21	0.60
1:A:406:GLN:O	1:A:410:ASP:N	2.31	0.60
2:B:41:LEU:O	2:B:43:LEU:N	2.35	0.59
1:A:223:GLU:OE2	2:B:241:SER:OG	2.20	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:ASP:HA	2:B:88:ASP:OD2	2.03	0.59
2:D:165:GLU:CD	2:D:198:GLN:HE22	2.05	0.59
2:D:104:GLN:HB3	2:D:220:SER:H	1.67	0.59
2:D:61:ILE:HG22	2:D:65:ARG:HD2	1.84	0.59
1:A:191:ASP:OD1	1:A:191:ASP:N	2.27	0.58
1:C:404:ASP:OD1	1:C:428:ARG:NH2	2.31	0.58
1:A:389:GLN:HG3	2:B:353:VAL:HG21	1.86	0.58
1:C:105:MET:O	1:C:109:ILE:HG12	2.03	0.58
2:B:287:GLU:O	2:B:290:THR:OG1	2.15	0.58
2:D:268:HIS:N	2:D:271:GLU:OE2	2.23	0.58
2:D:326:ILE:HG13	2:D:338:MET:HG2	1.84	0.58
1:A:179:VAL:HG12	1:A:186:VAL:HG22	1.86	0.58
1:C:189:VAL:O	1:C:201:GLN:NE2	2.33	0.58
1:A:132:LEU:HB3	2:B:33:VAL:HG21	1.84	0.57
2:B:32:GLU:O	2:B:36:GLU:HG3	2.03	0.57
1:A:116:VAL:HB	1:A:119:CYS:HB3	1.85	0.57
1:A:160:THR:HG22	1:A:162:GLN:H	1.68	0.57
1:C:342:ARG:HH12	1:C:344:GLN:HB2	1.70	0.57
1:C:446:PHE:HZ	2:D:290:THR:HB	1.69	0.57
2:D:199:VAL:HG22	2:D:222:LEU:HD13	1.86	0.57
1:A:210:TYR:CD1	1:A:218:VAL:HG13	2.39	0.57
1:A:387:GLN:N	1:A:390:GLU:OE1	2.25	0.57
1:C:214:HIS:HB2	1:C:266:ARG:HB2	1.85	0.57
2:B:101:VAL:HG13	2:B:109:ILE:CD1	2.34	0.56
2:D:296:LEU:HD13	2:D:302:VAL:HG22	1.87	0.56
1:A:380:CYS:SG	1:A:381:VAL:N	2.78	0.56
2:D:268:HIS:HB3	2:D:270:GLU:OE1	2.05	0.56
1:A:163:GLU:HG2	2:B:70:LEU:CD1	2.21	0.56
1:A:389:GLN:N	1:A:389:GLN:OE1	2.26	0.56
1:A:138:HIS:O	1:A:141:SER:HB3	2.05	0.56
1:A:189:VAL:HG13	1:A:201:GLN:HG3	1.88	0.56
1:C:200:PRO:HG2	1:C:203:GLU:HB2	1.88	0.56
1:C:426:MET:HG2	1:C:440:ARG:HB2	1.88	0.56
1:C:141:SER:OG	1:C:142:LEU:N	2.39	0.56
2:D:34:PHE:CD2	2:D:53:LYS:HD3	2.40	0.56
1:A:113:SER:O	1:A:120:SER:HB2	2.06	0.55
2:B:114:ASN:O	2:B:117:LYS:HB3	2.07	0.55
1:A:313:LYS:HG2	1:A:338:VAL:CG2	2.37	0.55
2:D:31:THR:HG22	2:D:53:LYS:NZ	2.21	0.55
1:A:379:ARG:O	1:A:383:THR:HG23	2.07	0.55
1:C:130:THR:O	1:C:133:ARG:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:328:ASN:HB3	2:D:331:ASN:OD1	2.07	0.55
1:C:261:ARG:HG3	2:D:238:PRO:HG2	1.88	0.55
1:A:130:THR:O	1:A:133:ARG:N	2.40	0.54
1:C:111:GLU:HA	1:C:114:ASP:OD2	2.08	0.54
1:A:201:GLN:O	1:A:205:PHE:N	2.29	0.54
2:B:286:SER:O	2:B:290:THR:HG23	2.08	0.54
2:B:101:VAL:HG12	2:B:110:PHE:HB3	1.90	0.54
2:B:354:PHE:N	2:B:358:GLN:OE1	2.35	0.54
2:D:134:PHE:HA	2:D:173:LYS:HD2	1.90	0.54
2:D:199:VAL:CG2	2:D:222:LEU:HD13	2.38	0.54
2:B:319:LEU:HD23	2:B:343:VAL:HA	1.89	0.54
1:C:161:ASP:OD1	1:C:161:ASP:N	2.41	0.54
1:C:397:VAL:O	1:C:400:CYS:HB3	2.07	0.54
1:A:313:LYS:HG2	1:A:338:VAL:HG23	1.88	0.53
2:D:241:SER:HA	2:D:260:ARG:NH1	2.23	0.53
2:B:92:LEU:HD21	2:B:113:GLU:HB3	1.90	0.53
1:C:129:LEU:O	1:C:133:ARG:HG3	2.08	0.53
2:B:122:THR:OG1	2:B:125:GLU:HG3	2.09	0.53
1:A:388:PRO:HB2	2:B:353:VAL:HG23	1.91	0.53
1:C:401:HIS:ND1	1:C:403:GLU:HG2	2.25	0.52
1:C:378:HIS:HB2	2:D:352:VAL:HG11	1.92	0.52
1:A:116:VAL:O	1:A:120:SER:N	2.32	0.52
1:C:266:ARG:HB3	1:C:303:PHE:HB3	1.91	0.52
1:C:366:ARG:HH21	2:D:283:ALA:HA	1.73	0.52
2:D:258:ASP:O	2:D:261:ILE:HG22	2.10	0.52
2:D:351:ASP:OD1	2:D:351:ASP:N	2.42	0.52
2:D:356:MET:O	2:D:359:THR:OG1	2.26	0.52
1:A:128:LYS:HD3	2:B:30:GLU:CD	2.29	0.52
2:B:38:ALA:O	2:B:48:SER:HB2	2.10	0.51
1:C:185:ARG:HD3	1:C:207:SER:O	2.11	0.51
2:D:163:SER:OG	2:D:165:GLU:OE1	2.26	0.51
1:A:380:CYS:HA	1:A:383:THR:OG1	2.11	0.51
2:B:260:ARG:HA	2:B:263:GLU:OE1	2.11	0.51
2:D:241:SER:C	2:D:243:THR:H	2.14	0.51
1:A:445:THR:HG22	1:A:447:GLN:NE2	2.25	0.51
2:B:247:ARG:HG2	2:B:248:HIS:N	2.24	0.51
1:C:418:LEU:HB3	1:C:421:GLN:OE1	2.11	0.51
2:D:247:ARG:HD2	2:D:336:CYS:SG	2.51	0.50
1:A:129:LEU:O	1:A:133:ARG:HG3	2.11	0.50
2:B:101:VAL:HA	2:B:222:LEU:O	2.11	0.50
1:A:179:VAL:HG12	1:A:186:VAL:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:VAL:HG23	1:A:197:LEU:HD12	1.93	0.50
1:A:414:GLN:HG3	1:A:418:LEU:HD13	1.93	0.50
1:C:381:VAL:HA	1:C:386:TYR:O	2.12	0.50
2:B:148:THR:O	2:B:166:ARG:NH2	2.43	0.50
1:C:175:PHE:HB2	1:C:192:SER:HB2	1.94	0.50
1:A:165:LYS:HB2	2:B:91:TYR:CZ	2.47	0.50
2:D:184:ASN:ND2	2:D:186:LYS:HB3	2.27	0.50
2:D:69:LEU:O	2:D:72:SER:HB3	2.12	0.49
2:D:92:LEU:HD21	2:D:112:SER:HB2	1.94	0.49
1:A:132:LEU:HB3	2:B:33:VAL:CG2	2.41	0.49
1:C:130:THR:O	1:C:134:MET:HG3	2.12	0.49
2:B:62:SER:HB3	2:B:109:ILE:O	2.13	0.49
2:D:47:VAL:HG23	2:D:48:SER:N	2.28	0.49
1:C:108:TYR:HB3	2:D:57:MET:HB3	1.93	0.49
1:C:116:VAL:O	1:C:120:SER:N	2.43	0.49
2:B:139:ASP:CG	2:B:171:ARG:HH21	2.15	0.48
1:C:178:ILE:HD12	1:C:188:TYR:HB3	1.95	0.48
1:C:108:TYR:HB3	2:D:57:MET:HE2	1.95	0.48
2:D:164:THR:CB	2:D:198:GLN:HE21	2.25	0.48
2:D:45:HIS:HA	2:D:48:SER:OG	2.13	0.48
2:B:101:VAL:HG13	2:B:109:ILE:HD11	1.95	0.48
1:A:130:THR:O	1:A:134:MET:HG3	2.13	0.48
1:A:132:LEU:O	1:A:136:VAL:HG23	2.14	0.48
2:B:315:GLY:HA2	2:B:354:PHE:HE1	1.79	0.48
1:C:172:ALA:HB1	1:C:342:ARG:CD	2.43	0.48
2:B:38:ALA:O	2:B:41:LEU:HB2	2.14	0.48
1:C:389:GLN:CG	2:D:353:VAL:HB	2.44	0.48
1:C:129:LEU:HD11	2:D:30:GLU:HB2	1.96	0.48
2:B:197:GLY:HA3	2:B:223:ILE:O	2.14	0.47
1:A:111:GLU:OE2	2:B:65:ARG:NH2	2.46	0.47
2:B:87:MET:HB2	2:B:90:LEU:HD12	1.94	0.47
1:C:217:ASP:O	1:C:220:LYS:HG2	2.15	0.47
1:A:413:GLN:HA	2:D:50:HIS:ND1	2.30	0.47
1:C:314:ALA:HA	1:C:335:PHE:HA	1.96	0.47
2:D:258:ASP:OD2	2:D:260:ARG:HB2	2.13	0.47
1:C:451:SER:HB3	2:D:251:ASP:HB3	1.97	0.47
1:A:445:THR:CG2	1:A:447:GLN:NE2	2.78	0.47
2:B:252:MET:HG2	2:B:293:HIS:NE2	2.30	0.47
1:C:99:ARG:HB2	1:C:102:ARG:HH21	1.80	0.47
2:D:164:THR:N	2:D:165:GLU:OE1	2.48	0.47
1:A:130:THR:HG22	1:A:134:MET:CG	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:PRO:HB2	1:A:203:GLU:H	1.80	0.47
1:C:456:TYR:HE1	1:C:458:ILE:HD11	1.79	0.47
2:D:237:ILE:HA	2:D:238:PRO:HD2	1.53	0.47
1:A:259:SER:HB2	1:A:261:ARG:HH21	1.80	0.47
2:B:69:LEU:CD2	2:B:101:VAL:HG21	2.45	0.47
1:A:366:ARG:HD2	1:A:456:TYR:CE1	2.50	0.46
1:C:119:CYS:HA	1:C:122:LEU:HG	1.95	0.46
1:C:434:ARG:HA	1:C:434:ARG:HD3	1.59	0.46
1:A:189:VAL:HG22	1:A:190:SER:O	2.15	0.46
2:D:26:ARG:HD2	2:D:27:ARG:H	1.79	0.46
1:A:105:MET:O	1:A:108:TYR:HB2	2.16	0.46
1:C:414:GLN:O	1:C:418:LEU:N	2.37	0.46
1:A:431:SER:HB3	1:A:437:LEU:HD11	1.98	0.46
1:C:175:PHE:HE2	1:C:189:VAL:HG23	1.81	0.46
2:B:328:ASN:HB3	2:B:331:ASN:OD1	2.16	0.46
1:A:366:ARG:HD2	1:A:456:TYR:CZ	2.51	0.46
1:C:369:ILE:H	1:C:369:ILE:HG13	1.59	0.46
2:B:96:GLU:O	2:B:228:PRO:HD2	2.16	0.45
2:D:68:LYS:O	2:D:71:SER:HB3	2.16	0.45
2:B:32:GLU:HG2	2:B:36:GLU:OE2	2.16	0.45
1:C:132:LEU:HB3	2:D:33:VAL:HG22	1.98	0.45
1:A:132:LEU:HD13	2:B:33:VAL:HG13	1.98	0.45
2:D:136:HIS:HA	2:D:137:PRO:HD3	1.85	0.45
1:A:160:THR:HG22	1:A:162:GLN:N	2.30	0.45
1:A:192:SER:HA	1:A:195:PRO:HD2	1.98	0.45
2:B:247:ARG:HB3	2:B:256:TYR:HB3	1.98	0.45
1:C:136:VAL:HG22	2:D:37:LEU:HA	1.97	0.45
2:B:230:GLN:NE2	2:B:237:ILE:HD12	2.31	0.45
2:B:252:MET:HG2	2:B:293:HIS:CE1	2.52	0.45
1:C:178:ILE:HD12	1:C:188:TYR:HD2	1.81	0.45
1:C:342:ARG:NH1	1:C:343:LEU:O	2.48	0.45
1:C:389:GLN:HG3	2:D:353:VAL:HB	1.98	0.45
1:C:447:GLN:OE1	1:C:447:GLN:N	2.49	0.45
1:C:167:LEU:HD23	1:C:167:LEU:HA	1.83	0.45
2:B:308:ARG:HA	2:B:317:VAL:O	2.16	0.45
1:A:165:LYS:HB2	2:B:91:TYR:CE2	2.52	0.45
2:D:326:ILE:HB	2:D:336:CYS:SG	2.56	0.45
2:D:61:ILE:O	2:D:65:ARG:HG3	2.15	0.45
2:D:265:ILE:HG22	2:D:267:TYR:CE2	2.51	0.45
2:D:319:LEU:HD23	2:D:343:VAL:HA	1.98	0.45
2:B:165:GLU:HA	2:B:198:GLN:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:34:PHE:CE1	2:D:53:LYS:HB3	2.52	0.45
1:A:268:ARG:HA	1:A:302:HIS:O	2.17	0.44
2:B:121:LEU:HD13	2:B:126:LEU:HD21	1.99	0.44
2:B:167:ASP:OD1	2:B:194:HIS:NE2	2.50	0.44
1:A:160:THR:HB	1:A:163:GLU:CB	2.33	0.44
1:C:383:THR:HG22	1:C:384:VAL:HG13	1.99	0.44
1:C:416:VAL:O	1:C:419:LYS:HG3	2.17	0.44
1:A:125:LYS:H	1:A:125:LYS:HG3	1.57	0.44
1:A:448:ASN:HA	1:A:449:PRO:HD3	1.83	0.44
2:B:271:GLU:OE2	2:B:312:LYS:NZ	2.51	0.44
1:C:208:THR:HG22	1:C:210:TYR:H	1.82	0.44
1:C:376:VAL:HG21	1:C:391:LEU:HB2	1.98	0.44
1:C:410:ASP:O	1:C:414:GLN:HG2	2.18	0.44
1:A:181:CYS:N	1:A:335:PHE:O	2.44	0.44
2:B:73:VAL:HG22	2:B:200:ARG:CZ	2.48	0.44
2:B:257:CYS:SG	2:B:261:ILE:HD13	2.58	0.44
2:B:54:ALA:O	2:B:57:MET:HB2	2.17	0.44
2:D:236:ASP:N	2:D:236:ASP:OD1	2.45	0.44
2:D:37:LEU:HD12	2:D:37:LEU:HA	1.79	0.44
1:A:307:HIS:HE1	1:A:344:GLN:OE1	2.01	0.44
1:C:171:ALA:HB2	2:D:223:ILE:HG22	2.00	0.44
2:D:34:PHE:CE2	2:D:53:LYS:HD3	2.53	0.44
1:A:344:GLN:NE2	3:A:503:HOH:O	2.32	0.44
1:A:163:GLU:HA	1:A:166:HIS:HB2	2.00	0.43
1:A:404:ASP:OD2	1:A:428:ARG:HD2	2.18	0.43
1:C:380:CYS:SG	1:C:381:VAL:N	2.90	0.43
2:B:38:ALA:HA	2:B:41:LEU:HD12	2.00	0.43
1:C:132:LEU:HB3	2:D:33:VAL:CG2	2.48	0.43
2:D:165:GLU:CG	2:D:198:GLN:HE22	2.31	0.43
1:A:193:VAL:HG22	1:A:199:GLN:HB3	2.01	0.43
1:A:363:PHE:HB2	1:A:377:ASP:OD1	2.18	0.43
2:D:101:VAL:HG23	2:D:110:PHE:HD2	1.84	0.43
2:D:144:ARG:O	2:D:148:THR:HG23	2.18	0.43
2:B:249:SER:OG	2:B:251:ASP:OD1	2.24	0.43
1:A:260:ARG:NH1	2:B:93:LYS:O	2.30	0.43
1:A:178:ILE:HA	1:A:337:LEU:O	2.18	0.43
2:B:101:VAL:CG1	2:B:109:ILE:HD11	2.49	0.43
1:A:363:PHE:HB3	1:A:383:THR:HG21	2.01	0.43
1:A:375:PHE:HA	2:B:354:PHE:O	2.19	0.43
2:B:258:ASP:O	2:B:261:ILE:HG22	2.18	0.43
1:C:376:VAL:HG11	1:C:391:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:GLY:HA2	1:A:342:ARG:HA	2.01	0.43
1:C:189:VAL:HG13	1:C:201:GLN:HG3	1.99	0.43
1:C:446:PHE:CZ	2:D:290:THR:HB	2.51	0.43
1:A:120:SER:C	1:A:122:LEU:H	2.21	0.42
2:B:95:LEU:HA	2:B:95:LEU:HD12	1.84	0.42
2:D:227:GLU:HA	2:D:228:PRO:HD2	1.91	0.42
1:C:259:SER:CB	1:C:261:ARG:HH12	2.31	0.42
1:A:199:GLN:HG2	1:A:204:TRP:HE1	1.84	0.42
2:B:149:LEU:C	2:B:166:ARG:HH22	2.22	0.42
1:C:182:GLU:HG2	1:C:183:THR:HG23	2.01	0.42
2:D:183:VAL:HG12	2:D:184:ASN:N	2.34	0.42
2:D:31:THR:HG22	2:D:53:LYS:HZ3	1.84	0.42
1:A:112:LEU:HA	1:A:112:LEU:HD23	1.81	0.42
1:C:365:SER:OG	1:C:459:CYS:HB2	2.19	0.42
1:A:433:THR:O	1:A:434:ARG:HB2	2.19	0.42
2:B:170:MET:HG2	2:B:195:CYS:SG	2.60	0.42
1:C:426:MET:HA	1:C:439:MET:O	2.19	0.42
1:C:189:VAL:HG22	1:C:190:SER:O	2.19	0.42
1:C:208:THR:CG2	1:C:210:TYR:HD2	2.32	0.42
1:A:130:THR:O	1:A:134:MET:N	2.53	0.42
1:C:174:GLY:HA2	1:C:341:GLY:O	2.20	0.42
1:C:371:GLY:HA2	1:C:412:PHE:CE2	2.54	0.42
2:B:248:HIS:HA	2:B:253:LYS:O	2.19	0.42
1:C:363:PHE:HB2	1:C:379:ARG:HG3	2.00	0.42
1:A:423:LEU:HD12	1:A:423:LEU:HA	1.75	0.42
2:B:195:CYS:HA	2:B:225:MET:O	2.19	0.42
2:B:101:VAL:CG1	2:B:109:ILE:CD1	2.97	0.41
1:A:441:THR:HA	1:A:460:THR:O	2.20	0.41
2:B:237:ILE:HA	2:B:238:PRO:HD2	1.56	0.41
2:D:314:GLY:HA3	2:D:350:ASN:O	2.20	0.41
1:C:132:LEU:HA	1:C:132:LEU:HD23	1.90	0.41
1:C:174:GLY:HA3	1:C:342:ARG:HB3	2.02	0.41
1:A:160:THR:HG22	1:A:161:ASP:N	2.35	0.41
2:D:310:LEU:HD23	2:D:316:TYR:HB3	2.01	0.41
2:B:253:LYS:HA	2:B:276:SER:HA	2.03	0.41
1:C:220:LYS:O	1:C:224:GLN:HG2	2.21	0.41
1:C:374:THR:HA	2:D:356:MET:HG3	2.02	0.41
1:A:422:VAL:HA	1:A:443:SER:O	2.21	0.41
1:C:136:VAL:HG22	2:D:37:LEU:CA	2.51	0.41
2:B:254:PHE:HB2	2:B:272:LEU:O	2.20	0.41
2:B:44:PRO:O	2:B:45:HIS:C	2.57	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:418:LEU:O	1:C:421:GLN:HG3	2.20	0.41
2:D:257:CYS:SG	2:D:261:ILE:HB	2.61	0.41
1:C:192:SER:O	1:C:196:VAL:HG23	2.21	0.41
1:A:221:LEU:O	1:A:225:LEU:HD13	2.20	0.41
1:A:426:MET:CE	1:A:464:VAL:HG21	2.51	0.41
1:A:164:LEU:O	1:A:168:ILE:HG12	2.20	0.41
2:B:93:LYS:HB2	2:B:93:LYS:HE3	1.78	0.41
2:B:33:VAL:HA	2:B:36:GLU:CG	2.51	0.40
2:B:39:HIS:CE1	2:B:45:HIS:HB2	2.57	0.40
2:B:38:ALA:HB1	2:B:48:SER:O	2.21	0.40
1:C:224:GLN:O	1:C:261:ARG:HD3	2.21	0.40
1:C:401:HIS:CE1	1:C:403:GLU:HG2	2.56	0.40
1:A:209:LEU:HA	1:A:209:LEU:HD12	1.81	0.40
2:B:59:LEU:HD21	2:B:124:VAL:HA	2.03	0.40
2:B:164:THR:O	2:B:199:VAL:N	2.40	0.40
1:A:396:ILE:HG12	1:A:408:LEU:HD21	2.04	0.40
2:B:244:PHE:HB2	2:B:258:ASP:OD1	2.20	0.40
1:C:389:GLN:HA	1:C:392:LEU:HD12	2.02	0.40
2:D:282:HIS:CB	2:D:308:ARG:HB2	2.51	0.40
2:B:183:VAL:HB	2:B:187:SER:HB2	2.03	0.40
1:C:175:PHE:CE2	1:C:189:VAL:HG23	2.57	0.40
1:C:199:GLN:HB3	1:C:199:GLN:HE21	1.72	0.40
2:D:133:ASP:O	2:D:173:LYS:HE2	2.21	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	249/384 (65%)	236 (95%)	13 (5%)	0	100	100
1	C	246/384 (64%)	234 (95%)	12 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	287/360 (80%)	275 (96%)	12 (4%)	0	100 | 100
2	D	278/360 (77%)	267 (96%)	11 (4%)	0	100 | 100
All	All	1060/1488 (71%)	1012 (96%)	48 (4%)	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	242/347 (70%)	240 (99%)	2 (1%)	85 | 91
1	C	239/347 (69%)	234 (98%)	5 (2%)	59 | 72
2	B	273/329 (83%)	271 (99%)	2 (1%)	87 | 93
2	D	267/329 (81%)	267 (100%)	0	100 | 100
All	All	1021/1352 (76%)	1012 (99%)	9 (1%)	82 | 90

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	161	ASP
1	A	164	LEU
2	B	45	HIS
2	B	357	ASP
1	C	204	TRP
1	C	302	HIS
1	C	342	ARG
1	C	434	ARG
1	C	456	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	447	GLN
1	C	387	GLN
1	C	447	GLN
2	D	198	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	261/384 (67%)	0.38	7 (2%)	55	65	44, 64, 94, 107	0
1	C	258/384 (67%)	0.25	5 (1%)	67	76	38, 64, 93, 116	0
2	B	295/360 (81%)	0.28	6 (2%)	65	75	37, 59, 94, 108	0
2	D	288/360 (80%)	0.28	9 (3%)	49	61	36, 58, 88, 104	0
All	All	1102/1488 (74%)	0.30	27 (2%)	58	68	36, 61, 93, 116	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	163	GLU	4.3
2	B	43	LEU	3.5
1	C	128	LYS	3.4
1	A	122	LEU	3.3
1	C	136	VAL	3.2
2	B	70	LEU	3.1
2	D	201	VAL	3.0
2	B	35	TYR	2.9
1	A	457	ILE	2.8
1	C	131	ILE	2.7
1	C	116	VAL	2.6
2	D	354	PHE	2.6
2	D	34	PHE	2.5
1	A	369	ILE	2.5
2	D	268	HIS	2.4
2	D	162	VAL	2.4
1	A	115	MET	2.3
2	D	310	LEU	2.3
2	B	170	MET	2.2
1	A	337	LEU	2.2
2	B	47	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	182	THR	2.1
2	D	126	LEU	2.1
1	A	135	ALA	2.1
2	B	41	LEU	2.0
1	C	115	MET	2.0
2	D	50	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.