



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2026 – 11:44 am BST

PDB ID : 32JC / pdb_000032jc
Title : Structure of the pathogenic variant T186R of Human SHMT2 in a distorted tetrameric conformation
Authors : Giardina, G.; Boumis, G.; Di Matteo, A.; Breccia, S.
Deposited on : 2026-07-11
Resolution : 3.07 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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

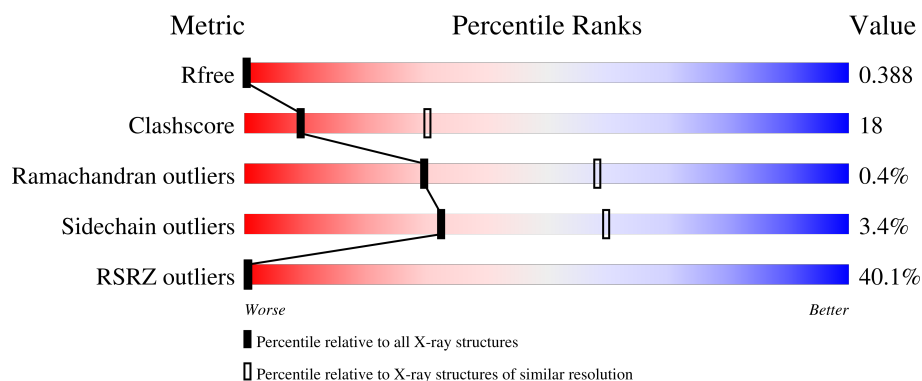
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.07 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	2010 (3.10-3.06)
Clashscore	190562	2102 (3.10-3.06)
Ramachandran outliers	187476	1982 (3.10-3.06)
Sidechain outliers	187428	1981 (3.10-3.06)
RSRZ outliers	180081	2010 (3.10-3.06)

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	486	22% 60% 28% 11%
1	B	486	49% 56% 30% 12%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6546 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 Serine hydroxymethyltransferase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	432	Total	C	N	O	S	0	0	0
			3270	2047	589	619	15			
1	B	426	Total	C	N	O	S	0	0	0
			3276	2067	590	605	14			

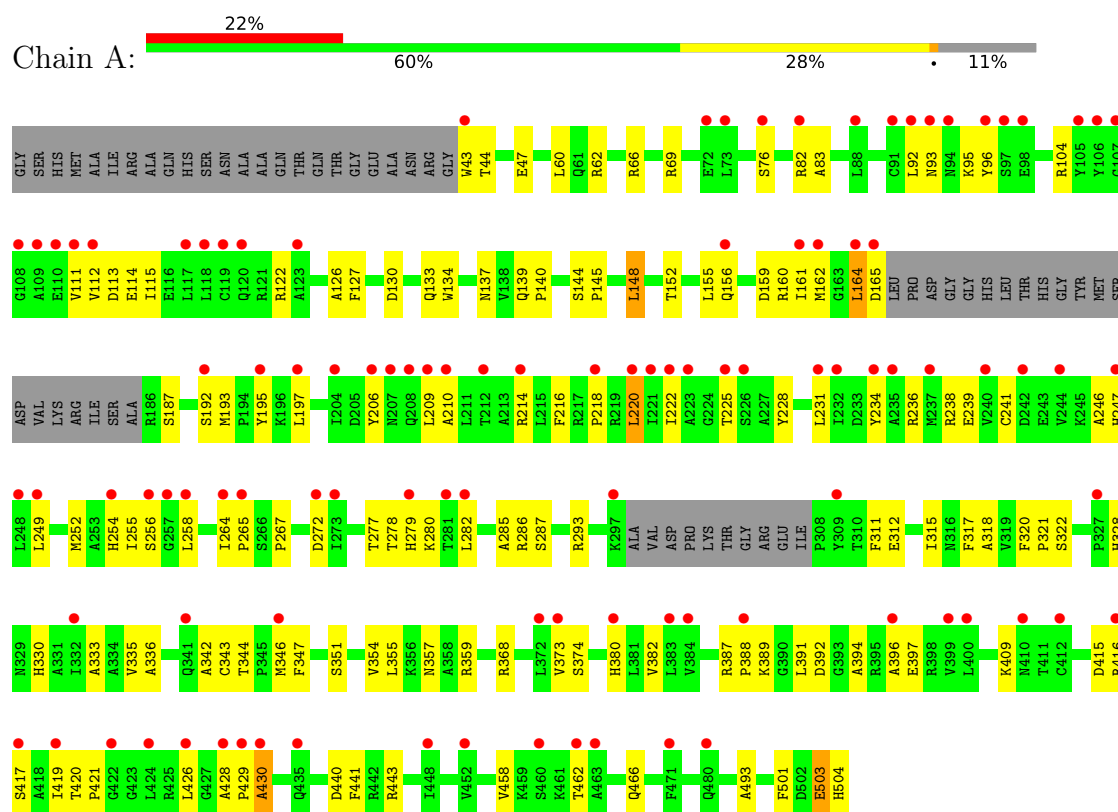
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	GLY	-	expression tag	UNP P34897
A	20	SER	-	expression tag	UNP P34897
A	21	HIS	-	expression tag	UNP P34897
A	186	ARG	THR	variant	UNP P34897
B	19	GLY	-	expression tag	UNP P34897
B	20	SER	-	expression tag	UNP P34897
B	21	HIS	-	expression tag	UNP P34897
B	186	ARG	THR	variant	UNP P34897

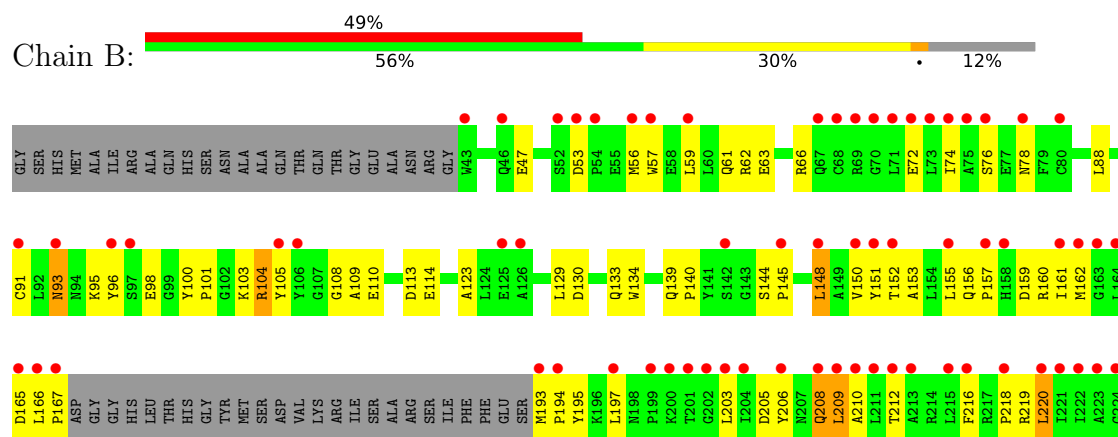
3 Residue-property plots

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: Serine hydroxymethyltransferase, mitochondrial



- Molecule 1: Serine hydroxymethyltransferase, mitochondrial





4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	160.41Å 160.41Å 206.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	80.33 – 3.07 80.33 – 3.07	Depositor EDS
% Data completeness (in resolution range)	78.3 (80.33-3.07) 78.3 (80.33-3.07)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 3.07Å)	Xtriage
Refinement program	REFMAC 5.8.0415	Depositor
R, R_{free}	0.351 , 0.389 0.348 , 0.388	Depositor DCC
R_{free} test set	1186 reflections (3.98%)	wwPDB-VP
Wilson B-factor (Å ²)	82.8	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 46.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	6546	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% 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	0.43	0/3329	0.83	0/4511
1	B	0.43	0/3336	0.82	0/4513
All	All	0.43	0/6665	0.82	0/9024

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3270	0	3164	117	6
1	B	3276	0	3264	137	6
All	All	6546	0	6428	235	6

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 18.

All (235) 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:299:VAL:HA	1:B:306:GLU:HA	1.51	0.93
1:A:122:ARG:NH2	1:B:53:ASP:OD1	2.00	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:LYS:HD2	1:A:421:PRO:HD2	1.53	0.88
1:B:144:SER:HB2	1:B:145:PRO:HD3	1.53	0.88
1:B:220:LEU:HD22	1:B:247:HIS:HB2	1.60	0.83
1:A:122:ARG:NH1	1:B:53:ASP:OD2	2.11	0.83
1:A:318:ALA:O	1:A:322:SER:HB2	1.80	0.81
1:A:155:LEU:HD11	1:A:220:LEU:HB2	1.66	0.77
1:B:130:ASP:HB3	1:B:133:GLN:HB2	1.67	0.76
1:A:429:PRO:O	1:A:430:ALA:CB	2.35	0.74
1:A:93:ASN:HD21	1:B:285:ALA:HA	1.52	0.74
1:B:357:ASN:HB3	1:B:441:PHE:CE2	2.22	0.74
1:A:114:GLU:OE1	1:B:62:ARG:NH2	2.21	0.72
1:A:160:ARG:HB3	1:A:216:PHE:CE2	2.26	0.70
1:A:139:GLN:N	1:A:140:PRO:CD	2.56	0.68
1:A:428:ALA:N	1:A:429:PRO:HD2	2.07	0.68
1:A:357:ASN:HB3	1:A:441:PHE:CD2	2.28	0.68
1:B:139:GLN:N	1:B:140:PRO:CD	2.57	0.68
1:B:249:LEU:HD11	1:B:275:THR:HG23	1.76	0.68
1:B:144:SER:HB2	1:B:145:PRO:CD	2.25	0.67
1:B:309:TYR:HD1	1:B:309:TYR:H	1.43	0.67
1:B:297:LYS:HB2	1:B:309:TYR:CG	2.30	0.66
1:B:95:LYS:HE3	1:B:108:GLY:O	1.95	0.66
1:A:417:SER:CB	1:A:421:PRO:HA	2.26	0.66
1:B:161:ILE:HG23	1:B:220:LEU:HB3	1.77	0.66
1:A:278:THR:OG1	1:A:285:ALA:O	2.14	0.66
1:A:126:ALA:HA	1:A:343:CYS:SG	2.36	0.65
1:B:428:ALA:N	1:B:429:PRO:CD	2.60	0.65
1:A:429:PRO:O	1:A:430:ALA:HB2	1.97	0.65
1:B:104:ARG:NE	1:B:113:ASP:OD1	2.24	0.64
1:A:164:LEU:HD23	1:A:195:TYR:CD1	2.33	0.64
1:A:43:TRP:CB	1:B:346:MET:HG3	2.28	0.64
1:A:134:TRP:CZ2	1:A:293:ARG:HD2	2.32	0.64
1:B:156:GLN:HB3	1:B:157:PRO:HD2	1.80	0.64
1:B:209:LEU:HD13	1:B:240:VAL:HG11	1.79	0.64
1:A:359:ARG:HG3	1:A:359:ARG:HH11	1.63	0.63
1:B:155:LEU:HD21	1:B:220:LEU:HB2	1.79	0.63
1:A:419:ILE:O	1:A:420:THR:OG1	2.15	0.63
1:B:162:MET:HE1	1:B:212:THR:HG23	1.80	0.62
1:A:220:LEU:HD23	1:A:247:HIS:HB2	1.82	0.62
1:A:387:ARG:HH11	1:A:415:ASP:HB2	1.63	0.61
1:A:137:ASN:OD1	1:A:140:PRO:HD3	2.00	0.61
1:A:164:LEU:O	1:A:165:ASP:O	2.19	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:ASN:ND2	1:B:93:ASN:O	2.34	0.61
1:A:164:LEU:HD23	1:A:195:TYR:CE1	2.36	0.61
1:B:104:ARG:HG3	1:B:105:TYR:H	1.66	0.61
1:A:373:VAL:O	1:A:374:SER:OG	2.16	0.60
1:B:257:GLY:HA3	1:B:281:THR:HB	1.83	0.60
1:B:299:VAL:C	1:B:301:PRO:HD3	2.26	0.60
1:B:134:TRP:CZ2	1:B:293:ARG:HD2	2.36	0.60
1:B:129:LEU:HD11	1:B:268:PHE:CE2	2.36	0.60
1:A:236:ARG:O	1:A:239:GLU:HB2	2.02	0.59
1:A:344:THR:OG1	1:A:346:MET:HE3	2.02	0.59
1:B:156:GLN:O	1:B:159:ASP:HB2	2.02	0.59
1:A:277:THR:HB	1:A:279:HIS:CE1	2.37	0.59
1:B:301:PRO:HG3	1:B:307:ILE:HD13	1.84	0.59
1:A:144:SER:HB2	1:A:145:PRO:HD3	1.85	0.58
1:B:458:VAL:HG12	1:B:458:VAL:O	2.03	0.58
1:A:258:LEU:HB2	1:A:264:ILE:HD11	1.86	0.58
1:B:96:TYR:HE1	1:B:98:GLU:HG3	1.69	0.58
1:B:263:VAL:HG23	1:B:264:ILE:HG23	1.84	0.58
1:B:346:MET:SD	1:B:346:MET:C	2.87	0.58
1:A:130:ASP:OD2	1:A:133:GLN:HG3	2.04	0.58
1:B:160:ARG:HD3	1:B:216:PHE:O	2.04	0.58
1:B:130:ASP:O	1:B:134:TRP:N	2.36	0.57
1:B:449:ASP:O	1:B:453:ASN:ND2	2.38	0.56
1:B:208:GLN:O	1:B:212:THR:HG22	2.05	0.56
1:A:278:THR:HG21	1:A:335:VAL:HG22	1.87	0.56
1:B:384:VAL:HG12	1:B:385:ASP:H	1.70	0.56
1:A:44:THR:HG22	1:B:435:GLN:HE22	1.70	0.56
1:A:346:MET:SD	1:A:346:MET:C	2.89	0.56
1:B:234:TYR:CZ	1:B:267:PRO:HB3	2.41	0.56
1:B:391:LEU:HG	1:B:392:ASP:H	1.70	0.56
1:A:104:ARG:NE	1:A:113:ASP:OD1	2.36	0.55
1:A:114:GLU:CD	1:B:62:ARG:HH22	2.13	0.55
1:A:328:HIS:HB3	1:A:330:HIS:CE1	2.41	0.55
1:B:428:ALA:H	1:B:429:PRO:HD3	1.71	0.55
1:B:387:ARG:HB2	1:B:388:PRO:HD3	1.88	0.55
1:B:197:LEU:HB2	1:B:203:LEU:O	2.07	0.55
1:A:317:PHE:HA	1:A:320:PHE:O	2.06	0.55
1:A:241:CYS:HB3	1:A:246:ALA:O	2.06	0.55
1:A:387:ARG:NH1	1:A:415:ASP:HB2	2.22	0.54
1:B:78:ASN:ND2	1:B:280:LYS:O	2.22	0.54
1:B:96:TYR:CE1	1:B:98:GLU:HG3	2.42	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:ARG:HH22	1:B:114:GLU:CD	2.15	0.54
1:A:164:LEU:O	1:A:165:ASP:C	2.51	0.54
1:A:428:ALA:H	1:A:429:PRO:HD2	1.73	0.54
1:B:151:TYR:O	1:B:155:LEU:HB2	2.08	0.54
1:A:357:ASN:HB3	1:A:441:PHE:CE2	2.43	0.54
1:B:167:PRO:HB3	1:B:194:PRO:HA	1.90	0.54
1:A:234:TYR:CE2	1:A:267:PRO:HB3	2.43	0.53
1:B:101:PRO:C	1:B:103:LYS:H	2.16	0.53
1:A:333:ALA:O	1:A:336:ALA:HB3	2.08	0.53
1:B:72:GLU:HA	1:B:406:THR:OG1	2.07	0.53
1:B:100:TYR:O	1:B:104:ARG:HG2	2.09	0.53
1:A:330:HIS:CD2	1:B:88:LEU:HD21	2.44	0.53
1:B:297:LYS:HB2	1:B:309:TYR:CD2	2.44	0.53
1:B:342:ALA:HA	1:B:347:PHE:CD2	2.44	0.52
1:A:387:ARG:N	1:A:388:PRO:CD	2.73	0.52
1:B:373:VAL:O	1:B:374:SER:OG	2.21	0.52
1:A:222:ILE:HG12	1:A:249:LEU:HD23	1.90	0.52
1:A:234:TYR:CZ	1:A:267:PRO:HB3	2.45	0.52
1:A:419:ILE:HG22	1:A:420:THR:HG23	1.91	0.52
1:B:167:PRO:HG3	1:B:194:PRO:HB3	1.92	0.52
1:A:111:VAL:HG11	1:B:63:GLU:HB2	1.92	0.52
1:B:458:VAL:HG13	1:B:471:PHE:CD1	2.45	0.52
1:A:228:TYR:HE2	1:A:231:LEU:O	1.92	0.51
1:A:417:SER:HB3	1:A:421:PRO:HA	1.90	0.51
1:B:318:ALA:O	1:B:322:SER:HB2	2.10	0.51
1:A:111:VAL:HB	1:B:63:GLU:OE1	2.10	0.51
1:A:225:THR:HG21	1:A:228:TYR:HB2	1.92	0.51
1:A:162:MET:HG3	1:A:218:PRO:HB3	1.92	0.51
1:A:264:ILE:HB	1:A:265:PRO:CD	2.40	0.51
1:B:129:LEU:HD21	1:B:268:PHE:CD2	2.45	0.51
1:B:148:LEU:O	1:B:152:THR:HG23	2.10	0.51
1:A:156:GLN:O	1:A:159:ASP:HB2	2.10	0.51
1:B:278:THR:OG1	1:B:285:ALA:O	2.24	0.51
1:B:428:ALA:N	1:B:429:PRO:HD3	2.26	0.51
1:A:95:LYS:HG2	1:A:112:VAL:HG21	1.93	0.50
1:A:320:PHE:CD1	1:A:321:PRO:HA	2.46	0.50
1:B:76:SER:O	1:B:280:LYS:HG2	2.11	0.50
1:B:357:ASN:HB3	1:B:441:PHE:CD2	2.47	0.50
1:A:69:ARG:O	1:A:493:ALA:HB3	2.12	0.50
1:A:368:ARG:O	1:A:389:LYS:NZ	2.44	0.50
1:B:150:VAL:HG11	1:B:249:LEU:HD22	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:TYR:O	1:B:354:VAL:HG23	2.11	0.50
1:A:466:GLN:HA	1:A:466:GLN:NE2	2.26	0.49
1:A:164:LEU:C	1:A:165:ASP:O	2.55	0.49
1:A:380:HIS:HB2	1:A:429:PRO:HD3	1.94	0.49
1:A:162:MET:HE3	1:A:193:MET:HG2	1.94	0.49
1:A:139:GLN:N	1:A:140:PRO:HD3	2.26	0.48
1:A:342:ALA:HA	1:A:347:PHE:CG	2.48	0.48
1:B:344:THR:OG1	1:B:346:MET:HE3	2.13	0.48
1:B:408:ASN:O	1:B:424:LEU:HD12	2.12	0.48
1:B:205:ASP:HB3	1:B:208:GLN:HE21	1.78	0.48
1:A:62:ARG:NH2	1:B:114:GLU:OE1	2.45	0.48
1:A:148:LEU:O	1:A:152:THR:HG23	2.14	0.48
1:A:258:LEU:HD13	1:A:355:LEU:HD21	1.95	0.48
1:B:328:HIS:HB3	1:B:330:HIS:CE1	2.48	0.48
1:A:139:GLN:H	1:A:140:PRO:HD3	1.79	0.48
1:A:336:ALA:CB	1:B:56:MET:HE3	2.43	0.48
1:A:76:SER:O	1:A:280:LYS:HG2	2.14	0.47
1:A:161:ILE:O	1:A:192:SER:HA	2.15	0.47
1:A:409:LYS:CD	1:A:421:PRO:HD2	2.35	0.47
1:A:311:PHE:O	1:A:312:GLU:C	2.56	0.47
1:B:104:ARG:HG3	1:B:105:TYR:N	2.30	0.47
1:B:209:LEU:C	1:B:209:LEU:HD22	2.40	0.47
1:A:336:ALA:HB3	1:B:56:MET:HE3	1.97	0.47
1:B:153:ALA:HB1	1:B:314:ARG:HB3	1.94	0.47
1:B:238:ARG:HH22	1:B:272:ASP:CG	2.22	0.47
1:B:96:TYR:CE1	1:B:326:GLY:HA3	2.49	0.47
1:A:346:MET:SD	1:A:347:PHE:N	2.88	0.47
1:A:380:HIS:HB2	1:A:429:PRO:CD	2.45	0.47
1:B:162:MET:HG2	1:B:195:TYR:OH	2.15	0.46
1:B:482:LEU:O	1:B:485:LEU:N	2.48	0.46
1:A:391:LEU:HG	1:A:392:ASP:H	1.80	0.46
1:B:458:VAL:O	1:B:458:VAL:CG1	2.63	0.46
1:A:111:VAL:CG1	1:B:63:GLU:HB2	2.46	0.46
1:A:206:TYR:HB3	1:A:236:ARG:HE	1.80	0.46
1:A:127:PHE:CE1	1:A:252:MET:HE1	2.51	0.46
1:B:139:GLN:N	1:B:140:PRO:HD3	2.31	0.45
1:A:238:ARG:HH22	1:A:272:ASP:CG	2.24	0.45
1:B:403:VAL:HG11	1:B:485:LEU:HD23	1.99	0.45
1:A:255:ILE:O	1:A:256:SER:C	2.59	0.45
1:A:187:SER:HB3	1:A:192:SER:OG	2.17	0.45
1:A:258:LEU:HB2	1:A:264:ILE:CD1	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:THR:HG21	1:B:382:VAL:HB	1.99	0.45
1:B:392:ASP:OD1	1:B:394:ALA:N	2.49	0.45
1:B:139:GLN:O	1:B:140:PRO:C	2.60	0.45
1:B:91:CYS:C	1:B:93:ASN:H	2.24	0.45
1:A:278:THR:HG21	1:A:335:VAL:CG2	2.48	0.44
1:B:206:TYR:O	1:B:209:LEU:HB3	2.17	0.44
1:B:148:LEU:HD22	1:B:152:THR:HG23	1.99	0.44
1:B:391:LEU:HD12	1:B:459:LYS:HD2	2.00	0.44
1:B:436:PHE:CE1	1:B:496:PHE:CD2	3.05	0.44
1:B:160:ARG:CB	1:B:218:PRO:HA	2.48	0.44
1:B:277:THR:HB	1:B:279:HIS:CE1	2.53	0.44
1:B:297:LYS:HD2	1:B:309:TYR:HB3	2.00	0.44
1:B:466:GLN:HA	1:B:466:GLN:NE2	2.32	0.44
1:B:209:LEU:HD13	1:B:240:VAL:HG21	2.00	0.44
1:B:72:GLU:OE2	1:B:74:ILE:HD12	2.18	0.43
1:A:394:ALA:HB2	1:A:420:THR:HA	2.00	0.43
1:A:501:PHE:HB2	1:A:504:HIS:OXT	2.17	0.43
1:B:91:CYS:C	1:B:93:ASN:N	2.75	0.43
1:B:123:ALA:HA	1:B:339:LEU:HD13	2.00	0.43
1:B:162:MET:SD	1:B:218:PRO:HG3	2.57	0.43
1:A:503:GLU:H	1:A:503:GLU:CD	2.26	0.43
1:B:302:LYS:HG2	1:B:303:THR:HG23	2.01	0.43
1:B:165:ASP:O	1:B:166:LEU:C	2.61	0.43
1:B:320:PHE:CD1	1:B:321:PRO:HA	2.53	0.43
1:A:92:LEU:HD11	1:A:115:ILE:HD13	2.01	0.43
1:A:285:ALA:O	1:A:287:SER:N	2.52	0.43
1:B:299:VAL:O	1:B:301:PRO:HD3	2.18	0.43
1:A:115:ILE:HA	1:B:59:LEU:HD13	2.01	0.43
1:A:210:ALA:O	1:A:214:ARG:HG3	2.17	0.43
1:A:382:VAL:CG2	1:A:426:LEU:HB2	2.49	0.43
1:B:342:ALA:HA	1:B:347:PHE:CG	2.54	0.43
1:B:365:LEU:O	1:B:370:TYR:HB2	2.19	0.43
1:A:160:ARG:HB2	1:A:218:PRO:HA	2.00	0.42
1:A:373:VAL:O	1:A:374:SER:CB	2.67	0.42
1:A:458:VAL:O	1:A:462:THR:OG1	2.15	0.42
1:A:82:ARG:O	1:A:83:ALA:C	2.62	0.42
1:A:134:TRP:CH2	1:A:293:ARG:HD2	2.54	0.42
1:A:359:ARG:HH11	1:A:359:ARG:CG	2.30	0.42
1:B:130:ASP:O	1:B:133:GLN:N	2.52	0.42
1:B:153:ALA:HB2	1:B:318:ALA:HB2	2.01	0.42
1:B:400:LEU:HA	1:B:403:VAL:HG22	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:SER:HB2	1:A:421:PRO:HA	1.99	0.42
1:A:66:ARG:HA	1:A:69:ARG:CZ	2.50	0.42
1:A:315:ILE:O	1:A:318:ALA:N	2.53	0.42
1:A:92:LEU:CD2	1:B:63:GLU:HG2	2.50	0.41
1:A:95:LYS:HD3	1:B:66:ARG:NH2	2.34	0.41
1:B:219:ARG:NH1	1:B:246:ALA:HA	2.35	0.41
1:B:234:TYR:CE1	1:B:267:PRO:HB3	2.55	0.41
1:B:152:THR:HG21	1:B:323:LEU:HD21	2.03	0.41
1:A:282:LEU:HD23	1:A:282:LEU:HA	1.84	0.41
1:B:484:ASN:OD1	1:B:488:ARG:NE	2.46	0.41
1:B:282:LEU:HD23	1:B:282:LEU:HA	1.91	0.41
1:B:408:ASN:O	1:B:424:LEU:CD1	2.69	0.41
1:B:160:ARG:HB2	1:B:218:PRO:HA	2.01	0.41
1:B:206:TYR:HB3	1:B:236:ARG:NH1	2.36	0.41
1:B:63:GLU:OE1	1:B:63:GLU:HA	2.21	0.41
1:A:104:ARG:HH21	1:A:113:ASP:HA	1.86	0.41
1:B:109:ALA:O	1:B:110:GLU:C	2.63	0.41
1:B:209:LEU:O	1:B:210:ALA:C	2.64	0.41
1:B:309:TYR:CD1	1:B:309:TYR:N	2.78	0.41
1:A:440:ASP:O	1:A:443:ARG:HB3	2.21	0.40
1:B:220:LEU:HD11	1:B:249:LEU:HB3	2.03	0.40
1:B:57:TRP:O	1:B:61:GLN:HG3	2.21	0.40
1:B:359:ARG:HH11	1:B:359:ARG:HG3	1.86	0.40
1:B:384:VAL:HG12	1:B:385:ASP:N	2.33	0.40
1:A:111:VAL:HG11	1:B:63:GLU:N	2.36	0.40
1:A:351:SER:O	1:A:354:VAL:HB	2.21	0.40
1:A:396:ALA:O	1:A:397:GLU:C	2.65	0.40
1:B:425:ARG:O	1:B:426:LEU:HD23	2.22	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:ARG:NH2	1:B:443:ARG:CZ[5_555]	1.24	0.96
1:A:236:ARG:NH2	1:B:443:ARG:NE[5_555]	1.40	0.80
1:A:416:ARG:NH2	1:B:453:ASN:OD1[8_665]	1.40	0.80
1:A:416:ARG:NH2	1:B:453:ASN:CG[8_665]	1.72	0.48
1:A:236:ARG:NH2	1:B:443:ARG:NH1[5_555]	1.83	0.37
1:A:236:ARG:NH2	1:B:443:ARG:NH2[5_555]	2.13	0.07

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	426/486 (88%)	385 (90%)	39 (9%)	2 (0%)	24	54
1	B	418/486 (86%)	375 (90%)	42 (10%)	1 (0%)	43	71
All	All	844/972 (87%)	760 (90%)	81 (10%)	3 (0%)	30	58

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	430	ALA
1	A	286	ARG
1	B	311	PHE

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	331/397 (83%)	321 (97%)	10 (3%)	36	62
1	B	338/397 (85%)	325 (96%)	13 (4%)	29	57
All	All	669/794 (84%)	646 (97%)	23 (3%)	32	60

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	GLU
1	A	60	LEU
1	A	96	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	148	LEU
1	A	164	LEU
1	A	197	LEU
1	A	209	LEU
1	A	220	LEU
1	A	254	HIS
1	A	503	GLU
1	B	47	GLU
1	B	93	ASN
1	B	104	ARG
1	B	148	LEU
1	B	193	MET
1	B	208	GLN
1	B	209	LEU
1	B	220	LEU
1	B	299	VAL
1	B	309	TYR
1	B	381	LEU
1	B	382	VAL
1	B	503	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	ASN
1	A	247	HIS
1	A	329	ASN
1	A	330	HIS
1	A	341	GLN
1	A	353	GLN
1	A	466	GLN
1	B	120	GLN
1	B	208	GLN
1	B	254	HIS
1	B	270	HIS
1	B	341	GLN
1	B	435	GLN
1	B	453	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 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

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(Å ²)	Q<0.9
1	A	432/486 (88%)	1.49	105 (24%) 2 1	51, 76, 110, 128	0
1	B	426/486 (87%)	2.32	239 (56%) 0 0	48, 101, 144, 150	0
All	All	858/972 (88%)	1.90	344 (40%) 0 0	48, 87, 134, 150	0

All (344) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	399	VAL	8.1
1	B	427	GLY	7.4
1	B	482	LEU	6.9
1	B	403	VAL	6.7
1	B	367	GLU	6.1
1	B	457	GLU	6.1
1	B	396	ALA	6.1
1	A	396	ALA	6.0
1	B	413	PRO	5.8
1	B	426	LEU	5.8
1	B	472	LEU	5.7
1	B	384	VAL	5.3
1	B	389	LYS	5.2
1	B	202	GLY	5.1
1	A	107	GLY	5.1
1	B	72	GLU	5.1
1	A	93	ASN	4.9
1	B	161	ILE	4.8
1	A	435	GLN	4.8
1	B	223	ALA	4.8
1	B	231	LEU	4.8
1	B	428	ALA	4.7
1	B	264	ILE	4.6
1	B	410	ASN	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	96	TYR	4.5
1	A	108	GLY	4.5
1	B	380	HIS	4.4
1	B	412	CYS	4.4
1	B	167	PRO	4.4
1	B	473	LEU	4.4
1	B	446	ASP	4.3
1	B	483	ALA	4.3
1	B	405	ILE	4.3
1	B	423	GLY	4.3
1	B	227	ALA	4.3
1	B	429	PRO	4.3
1	B	386	LEU	4.2
1	B	106	TYR	4.2
1	B	454	ILE	4.2
1	B	382	VAL	4.2
1	B	424	LEU	4.2
1	B	295	GLY	4.2
1	A	225	THR	4.1
1	B	447	PHE	4.1
1	B	240	VAL	4.1
1	B	468	PHE	4.1
1	B	422	GLY	4.1
1	B	369	GLY	4.0
1	B	390	GLY	4.0
1	B	222	ILE	4.0
1	B	400	LEU	4.0
1	A	273	ILE	3.9
1	B	379	ASN	3.9
1	B	359	ARG	3.9
1	B	150	VAL	3.9
1	A	76	SER	3.9
1	B	448	ILE	3.9
1	A	400	LEU	3.9
1	A	222	ILE	3.8
1	A	460	SER	3.8
1	B	485	LEU	3.8
1	A	195	TYR	3.8
1	B	281	THR	3.8
1	B	395	ARG	3.8
1	B	402	LEU	3.7
1	A	110	GLU	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	225	THR	3.7
1	B	453	ASN	3.7
1	B	71	LEU	3.7
1	B	163	GLY	3.7
1	B	216	PHE	3.7
1	B	478	THR	3.7
1	A	165	ASP	3.7
1	B	430	ALA	3.7
1	A	452	VAL	3.7
1	A	208	GLN	3.7
1	A	106	TYR	3.6
1	B	406	THR	3.6
1	B	355	LEU	3.6
1	B	391	LEU	3.6
1	B	311	PHE	3.6
1	B	374	SER	3.6
1	A	412	CYS	3.5
1	A	162	MET	3.5
1	A	204	ILE	3.5
1	A	380	HIS	3.5
1	B	407	ALA	3.5
1	B	226	SER	3.5
1	B	361	MET	3.5
1	B	234	TYR	3.4
1	A	209	LEU	3.4
1	B	381	LEU	3.4
1	B	272	ASP	3.4
1	A	399	VAL	3.4
1	B	248	LEU	3.4
1	B	75	ALA	3.4
1	B	388	PRO	3.4
1	B	479	SER	3.4
1	B	481	ARG	3.4
1	B	421	PRO	3.4
1	B	155	LEU	3.4
1	B	383	LEU	3.4
1	B	276	THR	3.4
1	B	435	GLN	3.4
1	B	74	ILE	3.3
1	B	307	ILE	3.3
1	B	378	ASP	3.3
1	B	289	LEU	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	206	TYR	3.3
1	B	105	TYR	3.3
1	A	119	CYS	3.3
1	B	442	ARG	3.3
1	A	223	ALA	3.3
1	B	200	LYS	3.2
1	B	56	MET	3.2
1	B	368	ARG	3.2
1	B	96	TYR	3.2
1	B	215	LEU	3.2
1	B	265	PRO	3.2
1	B	267	PRO	3.2
1	B	68	CYS	3.2
1	B	467	ASP	3.2
1	B	203	LEU	3.2
1	A	105	TYR	3.2
1	B	458	VAL	3.2
1	B	69	ARG	3.2
1	B	275	THR	3.2
1	A	297	LYS	3.2
1	B	73	LEU	3.1
1	A	234	TYR	3.1
1	B	266	SER	3.1
1	B	209	LEU	3.1
1	B	263	VAL	3.1
1	A	97	SER	3.1
1	B	224	GLY	3.1
1	B	274	VAL	3.1
1	B	425	ARG	3.1
1	B	151	TYR	3.1
1	A	383	LEU	3.1
1	B	249	LEU	3.1
1	B	325	GLY	3.1
1	B	411	THR	3.1
1	A	410	ASN	3.1
1	B	282	LEU	3.1
1	B	360	ALA	3.0
1	A	480	GLN	3.0
1	A	98	GLU	3.0
1	A	249	LEU	3.0
1	A	240	VAL	3.0
1	B	354	VAL	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	193	MET	3.0
1	B	76	SER	3.0
1	B	310	THR	3.0
1	A	192	SER	3.0
1	B	364	ALA	3.0
1	B	385	ASP	3.0
1	B	459	LYS	2.9
1	B	206	TYR	2.9
1	B	296	VAL	2.9
1	B	445	VAL	2.9
1	B	377	THR	2.9
1	B	431	LEU	2.9
1	A	309	TYR	2.9
1	B	220	LEU	2.9
1	B	373	VAL	2.9
1	B	97	SER	2.9
1	B	194	PRO	2.9
1	B	441	PHE	2.9
1	B	492	PHE	2.9
1	B	93	ASN	2.9
1	B	148	LEU	2.9
1	A	463	ALA	2.8
1	B	278	THR	2.8
1	B	78	ASN	2.8
1	B	59	LEU	2.8
1	B	197	LEU	2.8
1	B	308	PRO	2.8
1	B	211	LEU	2.8
1	B	372	LEU	2.8
1	B	324	GLN	2.8
1	B	213	ALA	2.8
1	B	235	ALA	2.8
1	B	158	HIS	2.8
1	A	237	MET	2.8
1	A	118	LEU	2.7
1	B	471	PHE	2.7
1	B	251	ASP	2.7
1	A	197	LEU	2.7
1	B	465	LEU	2.7
1	B	165	ASP	2.7
1	B	166	LEU	2.7
1	B	70	GLY	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	228	TYR	2.7
1	B	46	GLN	2.7
1	A	212	THR	2.7
1	A	109	ALA	2.7
1	B	164	LEU	2.7
1	A	341	GLN	2.6
1	A	429	PRO	2.6
1	B	142	SER	2.6
1	B	323	LEU	2.6
1	B	470	SER	2.6
1	A	117	LEU	2.6
1	A	210	ALA	2.6
1	B	254	HIS	2.6
1	B	54	PRO	2.6
1	B	436	PHE	2.6
1	A	272	ASP	2.6
1	B	366	LEU	2.6
1	B	409	LYS	2.6
1	B	464	LYS	2.6
1	A	264	ILE	2.6
1	B	80	CYS	2.6
1	A	281	THR	2.6
1	B	268	PHE	2.5
1	A	226	SER	2.5
1	A	156	GLN	2.5
1	B	257	GLY	2.5
1	B	456	LEU	2.5
1	A	244	VAL	2.5
1	B	440	ASP	2.5
1	B	210	ALA	2.5
1	B	250	ALA	2.5
1	A	327	PRO	2.5
1	A	282	LEU	2.5
1	B	404	SER	2.5
1	B	469	LYS	2.5
1	B	452	VAL	2.5
1	A	72	GLU	2.5
1	A	332	ILE	2.5
1	B	232	ILE	2.5
1	A	372	LEU	2.5
1	A	207	ASN	2.5
1	B	255	ILE	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	237	MET	2.5
1	A	218	PRO	2.5
1	A	221	ILE	2.5
1	B	125	GLU	2.5
1	B	152	THR	2.5
1	A	88	LEU	2.5
1	B	199	PRO	2.5
1	B	455	GLY	2.5
1	A	242	ASP	2.4
1	A	220	LEU	2.4
1	A	265	PRO	2.4
1	A	235	ALA	2.4
1	A	161	ILE	2.4
1	B	277	THR	2.4
1	A	388	PRO	2.4
1	A	111	VAL	2.4
1	B	444	VAL	2.4
1	B	229	ALA	2.4
1	B	212	THR	2.4
1	B	242	ASP	2.4
1	A	120	GLN	2.4
1	A	256	SER	2.4
1	A	43	TRP	2.4
1	A	91	CYS	2.4
1	A	254	HIS	2.3
1	A	430	ALA	2.3
1	A	73	LEU	2.3
1	A	92	LEU	2.3
1	B	347	PHE	2.3
1	B	397	GLU	2.3
1	B	201	THR	2.3
1	B	269	LYS	2.3
1	A	428	ALA	2.3
1	B	290	ILE	2.3
1	B	298	ALA	2.3
1	A	164	LEU	2.3
1	A	373	VAL	2.3
1	A	82	ARG	2.3
1	B	370	TYR	2.3
1	A	231	LEU	2.3
1	A	426	LEU	2.3
1	B	53	ASP	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	363	ASP	2.3
1	B	305	ARG	2.3
1	B	252	MET	2.3
1	A	258	LEU	2.3
1	B	365	LEU	2.3
1	B	466	GLN	2.3
1	A	416	ARG	2.3
1	B	398	ARG	2.3
1	A	123	ALA	2.3
1	B	52	SER	2.3
1	B	157	PRO	2.2
1	B	43	TRP	2.2
1	A	422	GLY	2.2
1	A	424	LEU	2.2
1	B	304	GLY	2.2
1	A	247	HIS	2.2
1	A	384	VAL	2.2
1	B	244	VAL	2.2
1	B	67	GLN	2.2
1	A	94	ASN	2.2
1	A	448	ILE	2.2
1	B	221	ILE	2.2
1	B	204	ILE	2.2
1	B	273	ILE	2.2
1	B	258	LEU	2.2
1	B	262	LYS	2.2
1	B	162	MET	2.2
1	B	493	ALA	2.2
1	A	257	GLY	2.2
1	B	321	PRO	2.2
1	B	376	GLY	2.2
1	B	439	ASP	2.2
1	B	57	TRP	2.2
1	B	247	HIS	2.2
1	B	432	THR	2.1
1	A	279	HIS	2.1
1	A	232	ILE	2.1
1	A	346	MET	2.1
1	B	351	SER	2.1
1	B	371	SER	2.1
1	B	408	ASN	2.1
1	B	270	HIS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	462	THR	2.1
1	B	253	ALA	2.1
1	B	145	PRO	2.1
1	A	417	SER	2.1
1	B	283	ARG	2.1
1	B	443	ARG	2.1
1	B	271	ALA	2.1
1	B	480	GLN	2.1
1	A	214	ARG	2.1
1	B	449	ASP	2.1
1	B	126	ALA	2.1
1	A	248	LEU	2.0
1	B	486	ARG	2.0
1	B	91	CYS	2.0
1	B	246	ALA	2.0
1	B	358	ALA	2.0
1	B	495	ALA	2.0
1	A	471	PHE	2.0
1	B	208	GLN	2.0
1	B	353	GLN	2.0
1	A	112	VAL	2.0
1	B	233	ASP	2.0
1	B	218	PRO	2.0
1	B	387	ARG	2.0
1	A	419	ILE	2.0
1	B	315	ILE	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.