



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:18 AM UTC

PDB ID : 2RAD / pdb_00002rad
Title : Crystal structure of the succinoglycan biosynthesis protein. Northeast structural Genomics Consortium target BcR135
Authors : Kuzin, A.P.; Abashidze, M.; Seetharaman, J.; Wang, H.; Mao, L.; Cunningham, K.; Xiao, R.; Liu, J.; Baran, M.C.; Acton, T.B.; Rost, B.; Montelione, G.T.; Tong, L.; Hunt, J.F.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2007-09-14
Resolution : 2.75 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
Mogul	:	2022.3.0, CSD as543be (2022)
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)

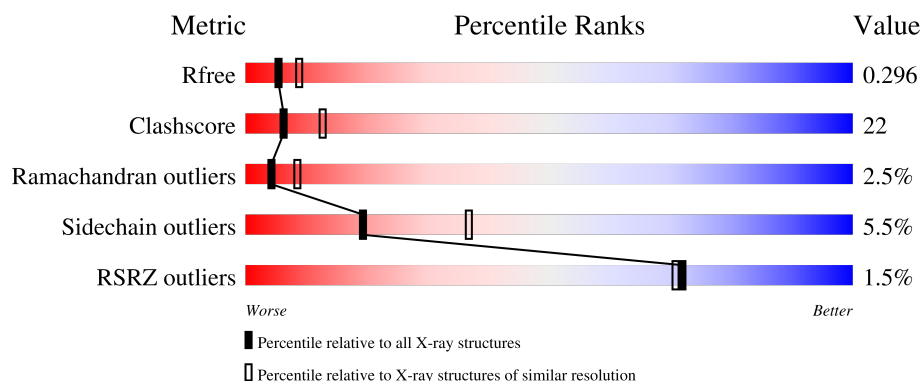
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	451	
1	B	451	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6506 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 Succinoglycan biosynthesis protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	403	Total	C	N	O	Se	0	0	0
			3230	2071	547	604	8			
1	B	405	Total	C	N	O	Se	0	0	0
			3245	2079	550	608	8			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	233	THR	GLN	conflict	UNP Q81BN2
A	444	LEU	-	expression tag	UNP Q81BN2
A	445	GLU	-	expression tag	UNP Q81BN2
A	446	HIS	-	expression tag	UNP Q81BN2
A	447	HIS	-	expression tag	UNP Q81BN2
A	448	HIS	-	expression tag	UNP Q81BN2
A	449	HIS	-	expression tag	UNP Q81BN2
A	450	HIS	-	expression tag	UNP Q81BN2
A	451	HIS	-	expression tag	UNP Q81BN2
B	233	THR	GLN	conflict	UNP Q81BN2
B	444	LEU	-	expression tag	UNP Q81BN2
B	445	GLU	-	expression tag	UNP Q81BN2
B	446	HIS	-	expression tag	UNP Q81BN2
B	447	HIS	-	expression tag	UNP Q81BN2
B	448	HIS	-	expression tag	UNP Q81BN2
B	449	HIS	-	expression tag	UNP Q81BN2
B	450	HIS	-	expression tag	UNP Q81BN2
B	451	HIS	-	expression tag	UNP Q81BN2

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	21	Total	O	0	0
			21	21		

Continued on next page...

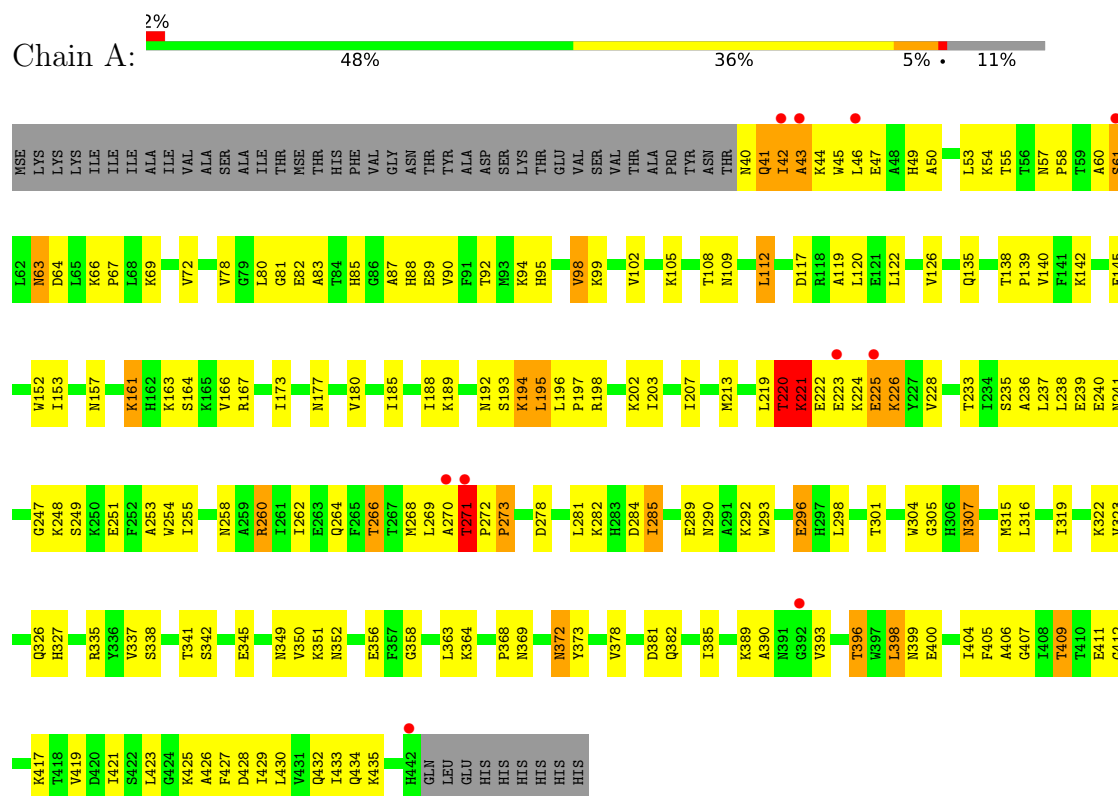
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	10	Total	O	0	0
			10	10		

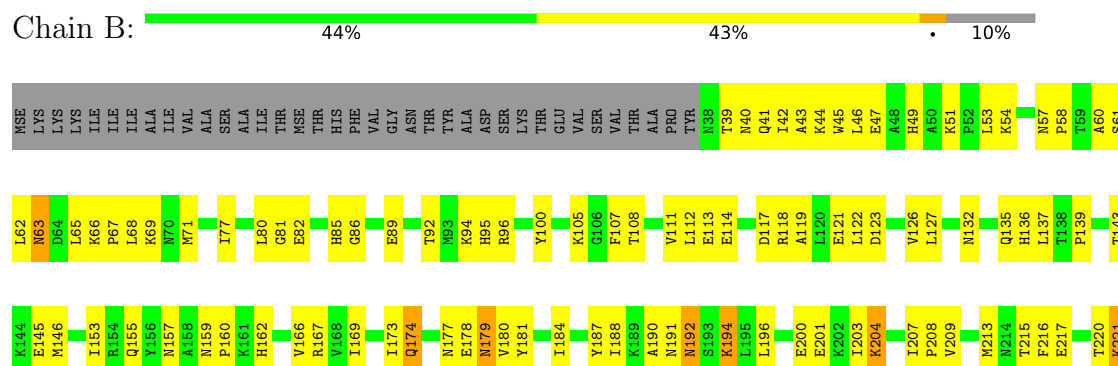
3 Residue-property plots

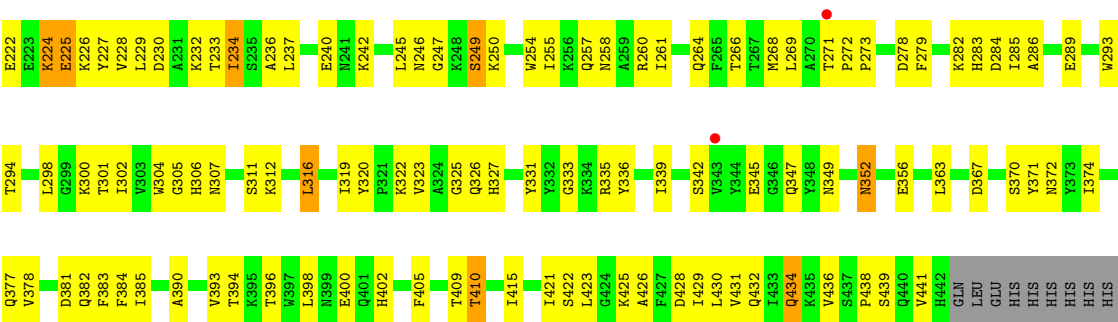
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Succinoglycan biosynthesis protein



• Molecule 1: Succinoglycan biosynthesis protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	87.79Å 54.19Å 98.91Å 90.00° 97.20° 90.00°	Depositor
Resolution (Å)	19.93 – 2.75 19.93 – 2.75	Depositor EDS
% Data completeness (in resolution range)	82.1 (19.93-2.75) 91.1 (19.93-2.75)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 2.77Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.209 , 0.281 0.225 , 0.296	Depositor DCC
R_{free} test set	4462 reflections (9.76%)	wwPDB-VP
Wilson B-factor (Å ²)	50.6	Xtriage
Anisotropy	0.726	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 38.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6506	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.21% 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

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	0.52	0/3298	1.03	22/4450 (0.5%)
1	B	0.49	0/3313	1.02	12/4471 (0.3%)
All	All	0.51	0/6611	1.02	34/8921 (0.4%)

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	43	ALA	N-CA-C	-11.97	97.44	112.88
1	B	234	ILE	N-CA-C	-8.83	102.23	110.53
1	B	66	LYS	CA-C-N	-8.07	111.91	119.82
1	B	66	LYS	C-N-CA	-8.07	111.91	119.82
1	A	43	ALA	N-CA-C	-7.90	103.20	112.92
1	A	222	GLU	N-CA-C	-7.42	102.89	110.97
1	A	221	LYS	N-CA-C	-7.41	104.39	113.50
1	B	40	ASN	N-CA-C	-6.79	104.87	113.02
1	A	42	ILE	N-CA-C	6.59	117.19	106.72
1	B	434	GLN	N-CA-C	6.55	119.24	111.71
1	A	253	ALA	N-CA-C	-6.39	104.23	111.07
1	B	44	LYS	N-CA-C	-6.25	104.72	112.90
1	B	113	GLU	N-CA-C	-6.02	102.31	110.68
1	A	393	VAL	N-CA-C	-6.01	104.65	110.72
1	A	296	GLU	N-CA-C	5.95	118.55	111.71
1	A	417	LYS	N-CA-C	-5.88	106.08	113.72
1	A	98	VAL	N-CA-C	-5.83	104.83	110.72
1	B	174	GLN	N-CA-C	-5.76	106.20	113.18
1	A	301	THR	N-CA-C	5.75	118.84	109.24
1	A	335	ARG	N-CA-C	-5.69	106.30	113.18
1	A	412	GLY	CA-C-N	5.56	125.66	119.32
1	A	412	GLY	C-N-CA	5.56	125.66	119.32
1	A	249	SER	N-CA-C	5.44	117.70	110.53
1	A	57	ASN	CA-C-N	5.38	124.83	119.24
1	A	57	ASN	C-N-CA	5.38	124.83	119.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	372	ASN	N-CA-C	5.34	117.10	111.28
1	B	250	LYS	N-CA-C	-5.31	106.97	113.50
1	A	285	ILE	N-CA-C	-5.30	104.46	111.09
1	A	271	THR	N-CA-C	-5.13	98.48	109.81
1	A	72	VAL	N-CA-C	-5.09	104.92	112.04
1	A	195	LEU	N-CA-C	-5.08	106.93	113.23
1	B	428	ASP	N-CA-C	-5.08	106.77	113.12
1	A	78	VAL	N-CA-C	5.08	115.29	107.77
1	B	284	ASP	N-CA-C	5.07	118.73	112.54

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	3230	0	3239	140	0
1	B	3245	0	3252	149	0
2	A	21	0	0	1	0
2	B	10	0	0	0	0
All	All	6506	0	6491	289	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 22.

All (289) 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:323:VAL:H	1:A:326:GLN:HE21	1.14	0.95
1:B:67:PRO:HG2	1:B:384:PHE:HZ	1.31	0.94
1:B:372:ASN:HD21	1:B:405:PHE:H	1.00	0.92
1:A:372:ASN:HD21	1:A:405:PHE:H	1.19	0.91
1:B:268:MSE:HE3	1:B:269:LEU:HG	1.56	0.88
1:A:285:ILE:O	1:A:289:GLU:HG3	1.77	0.85
1:B:221:LYS:HE3	1:B:224:LYS:HB2	1.61	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:SER:HB3	1:B:432:GLN:HE22	1.44	0.80
1:A:268:MSE:HG3	1:A:269:LEU:HD12	1.62	0.80
1:B:372:ASN:HD21	1:B:405:PHE:N	1.78	0.79
1:B:60:ALA:HB3	1:B:96:ARG:NH2	1.97	0.79
1:B:67:PRO:HG2	1:B:384:PHE:CZ	2.18	0.78
1:A:345:GLU:O	1:A:435:LYS:HA	1.84	0.78
1:B:47:GLU:HG2	1:B:378:VAL:HG13	1.66	0.78
1:A:188:ILE:HD11	1:A:238:LEU:HD21	1.66	0.78
1:A:202:LYS:HE3	1:A:233:THR:HG21	1.66	0.77
1:A:323:VAL:H	1:A:326:GLN:NE2	1.81	0.77
1:A:423:LEU:HD21	1:A:430:LEU:HD13	1.65	0.77
1:A:262:ILE:O	1:A:266:THR:HB	1.86	0.75
1:B:374:ILE:HD12	1:B:374:ILE:H	1.51	0.75
1:A:352:ASN:HD21	1:A:356:GLU:HB3	1.53	0.74
1:B:233:THR:HA	1:B:236:ALA:HB3	1.69	0.73
1:B:372:ASN:ND2	1:B:405:PHE:H	1.83	0.73
1:A:350:VAL:HG21	1:A:411:GLU:HG3	1.72	0.72
1:B:423:LEU:HD21	1:B:430:LEU:HD13	1.72	0.72
1:B:342:SER:HB3	1:B:432:GLN:NE2	2.04	0.71
1:A:196:LEU:HB3	1:A:197:PRO:HD3	1.73	0.70
1:B:228:VAL:HG22	1:B:266:THR:HG22	1.74	0.69
1:B:228:VAL:HA	1:B:266:THR:HG21	1.75	0.69
1:A:94:LYS:HZ1	1:A:304:TRP:CD1	2.11	0.68
1:B:221:LYS:NZ	1:B:221:LYS:HA	2.09	0.68
1:A:41:GLN:HB3	1:A:42:ILE:HD12	1.75	0.68
1:B:213:MSE:HG2	1:B:269:LEU:HD11	1.76	0.68
1:A:157:ASN:HD21	1:A:166:VAL:H	1.42	0.67
1:B:157:ASN:HD21	1:B:166:VAL:H	1.41	0.67
1:B:349:ASN:ND2	1:B:438:PRO:HB3	2.09	0.67
1:B:367:ASP:HB3	1:B:370:SER:HB3	1.77	0.67
1:B:312:LYS:HB2	1:B:425:LYS:O	1.95	0.66
1:B:41:GLN:NE2	1:B:42:ILE:HG12	2.10	0.66
1:A:264:GLN:HE22	1:A:290:ASN:HD21	1.42	0.66
1:A:396:THR:O	1:A:400:GLU:HG3	1.96	0.65
1:A:399:ASN:HD22	1:A:425:LYS:HE3	1.62	0.65
1:B:194:LYS:H	1:B:194:LYS:HD3	1.61	0.65
1:A:372:ASN:HD21	1:A:405:PHE:N	1.91	0.65
1:A:94:LYS:HZ1	1:A:304:TRP:CG	2.14	0.65
1:B:80:LEU:HG	1:B:94:LYS:HD2	1.80	0.64
1:B:312:LYS:O	1:B:326:GLN:HG2	1.98	0.64
1:B:349:ASN:HD21	1:B:438:PRO:HB3	1.63	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ALA:HA	1:A:46:LEU:HD13	1.78	0.64
1:B:126:VAL:HB	1:B:153:ILE:HG22	1.80	0.64
1:A:41:GLN:CB	1:A:42:ILE:HD12	2.29	0.63
1:A:82:GLU:OE2	1:A:85:HIS:HD2	1.81	0.63
1:A:272:PRO:HD3	1:A:282:LYS:HZ1	1.63	0.63
1:A:80:LEU:HG	1:A:94:LYS:HE3	1.81	0.63
1:B:221:LYS:HA	1:B:221:LYS:HZ1	1.63	0.63
1:B:132:ASN:ND2	1:B:135:GLN:HG2	2.14	0.62
1:A:83:ALA:O	1:A:407:GLY:HA3	1.99	0.62
1:A:138:THR:HG23	1:A:139:PRO:HD2	1.81	0.62
1:A:45:TRP:CZ3	1:A:385:ILE:HD11	2.34	0.62
1:A:47:GLU:HG2	1:A:378:VAL:HG13	1.82	0.62
1:B:246:ASN:ND2	1:B:249:SER:HB2	2.14	0.61
1:A:272:PRO:HD3	1:A:282:LYS:NZ	2.15	0.61
1:B:192:ASN:ND2	1:B:194:LYS:HG2	2.15	0.61
1:A:54:LYS:HE2	1:A:55:THR:HG22	1.82	0.61
1:A:81:GLY:HA2	1:A:305:GLY:O	2.01	0.60
1:A:432:GLN:C	1:A:433:ILE:HD12	2.27	0.60
1:B:180:VAL:HG13	1:B:258:ASN:HD22	1.66	0.60
1:B:260:ARG:O	1:B:264:GLN:HG3	2.01	0.60
1:B:319:ILE:HG13	1:B:320:TYR:N	2.15	0.60
1:A:271:THR:O	1:A:273:PRO:HD3	2.02	0.59
1:A:421:ILE:HD11	1:A:426:ALA:CB	2.31	0.59
1:B:285:ILE:O	1:B:289:GLU:HG3	2.02	0.59
1:B:209:VAL:O	1:B:216:PHE:HB2	2.02	0.59
1:B:319:ILE:HG13	1:B:320:TYR:H	1.67	0.59
1:B:187:TYR:CG	1:B:255:ILE:HG13	2.38	0.58
1:B:143:THR:HG22	1:B:441:VAL:HA	1.86	0.58
1:A:264:GLN:HE22	1:A:290:ASN:ND2	2.01	0.57
1:B:196:LEU:O	1:B:196:LEU:HD13	2.05	0.57
1:B:396:THR:O	1:B:400:GLU:HG3	2.05	0.57
1:A:46:LEU:O	1:A:50:ALA:HB2	2.04	0.57
1:A:69:LYS:HA	1:A:105:LYS:HE2	1.86	0.56
1:B:383:PHE:CE1	1:B:432:GLN:HB3	2.41	0.56
1:A:108:THR:O	1:A:166:VAL:HA	2.05	0.56
1:A:161:LYS:HE3	1:A:163:LYS:HZ2	1.70	0.56
1:B:41:GLN:CD	1:B:42:ILE:HG12	2.31	0.56
1:A:126:VAL:HB	1:A:153:ILE:HG22	1.88	0.56
1:A:350:VAL:HG23	1:A:409:THR:O	2.04	0.56
1:A:92:THR:O	1:A:95:HIS:HB3	2.05	0.56
1:B:86:GLY:C	1:B:439:SER:HB2	2.31	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:THR:O	1:B:166:VAL:HA	2.05	0.55
1:A:61:SER:OG	1:A:63:ASN:HB2	2.06	0.55
1:B:381:ASP:O	1:B:434:GLN:HG2	2.07	0.55
1:A:88:HIS:HA	1:A:145:GLU:OE2	2.07	0.55
1:B:278:ASP:O	1:B:282:LYS:HG2	2.07	0.55
1:B:311:SER:O	1:B:325:GLY:HA3	2.07	0.55
1:A:260:ARG:O	1:A:264:GLN:HG3	2.08	0.54
1:B:94:LYS:HZ1	1:B:304:TRP:CD1	2.25	0.54
1:B:107:PHE:CD2	1:B:300:LYS:HB3	2.43	0.54
1:A:195:LEU:HD11	1:A:241:ASN:CG	2.33	0.54
1:B:60:ALA:HB3	1:B:96:ARG:CZ	2.37	0.54
1:B:89:GLU:OE1	1:B:89:GLU:N	2.41	0.54
1:A:219:LEU:O	1:A:220:THR:HG23	2.07	0.53
1:A:82:GLU:HA	1:A:341:THR:OG1	2.08	0.53
1:B:112:LEU:HD23	1:B:304:TRP:HB3	1.89	0.53
1:B:204:LYS:HB2	1:B:204:LYS:NZ	2.24	0.53
1:B:381:ASP:HB3	1:B:382:GLN:NE2	2.25	0.52
1:A:46:LEU:HD12	1:A:46:LEU:H	1.74	0.52
1:B:81:GLY:HA3	1:B:307:ASN:HD22	1.74	0.52
1:B:236:ALA:O	1:B:240:GLU:HG2	2.10	0.52
1:B:410:THR:HG23	1:B:415:ILE:HD13	1.90	0.52
1:B:61:SER:OG	1:B:63:ASN:HB2	2.09	0.52
1:B:294:THR:HG23	1:B:298:LEU:HD12	1.91	0.52
1:A:223:GLU:HG3	1:A:224:LYS:H	1.75	0.52
1:A:109:ASN:HD21	1:A:298:LEU:HB3	1.74	0.51
1:A:260:ARG:HH21	1:A:289:GLU:HB3	1.76	0.51
1:A:173:ILE:HD12	1:A:268:MSE:HE2	1.92	0.51
1:A:342:SER:HB3	1:A:432:GLN:NE2	2.26	0.51
1:A:161:LYS:HE3	1:A:161:LYS:HA	1.93	0.51
1:A:322:LYS:HA	1:A:326:GLN:HE22	1.76	0.51
1:B:77:ILE:HG23	1:B:336:TYR:HD1	1.75	0.51
1:B:137:LEU:HD21	1:B:146:MSE:HE2	1.92	0.51
1:A:271:THR:HB	1:A:272:PRO:HD3	1.92	0.51
1:A:213:MSE:HA	1:A:269:LEU:HD21	1.92	0.51
1:A:372:ASN:ND2	1:A:405:PHE:H	2.00	0.51
1:A:138:THR:O	1:A:139:PRO:C	2.54	0.50
1:A:221:LYS:NZ	1:A:221:LYS:HB2	2.26	0.50
1:A:264:GLN:NE2	1:A:290:ASN:HD21	2.07	0.50
1:B:230:ASP:O	1:B:234:ILE:HG13	2.10	0.50
1:A:223:GLU:HB2	1:A:270:ALA:CB	2.42	0.50
1:B:203:ILE:HD12	1:B:204:LYS:N	2.26	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:GLU:O	1:A:255:ILE:HG12	2.11	0.50
1:A:271:THR:N	1:A:272:PRO:HD2	2.26	0.50
1:A:337:VAL:HA	1:A:428:ASP:OD2	2.11	0.50
1:A:433:ILE:HD12	1:A:433:ILE:N	2.27	0.50
1:A:95:HIS:C	1:A:95:HIS:CD2	2.90	0.50
1:B:301:THR:HG22	1:B:302:ILE:N	2.27	0.50
1:A:223:GLU:O	1:A:228:VAL:HG23	2.11	0.49
1:A:271:THR:N	1:A:272:PRO:CD	2.75	0.49
1:B:178:GLU:HA	1:B:181:TYR:HD2	1.77	0.49
1:B:194:LYS:HD3	1:B:194:LYS:N	2.26	0.49
1:A:46:LEU:HD12	1:A:46:LEU:N	2.28	0.49
1:B:39:THR:C	1:B:41:GLN:H	2.20	0.49
1:B:390:ALA:HB1	1:B:394:THR:HG22	1.94	0.49
1:B:121:GLU:HG3	1:B:136:HIS:CE1	2.47	0.49
1:B:240:GLU:C	1:B:242:LYS:H	2.20	0.49
1:A:49:HIS:HD2	1:A:389:LYS:HE3	1.77	0.49
1:A:87:ALA:HB3	1:A:90:VAL:HG23	1.95	0.49
1:B:58:PRO:HA	1:B:96:ARG:HG2	1.94	0.49
1:A:349:ASN:HA	1:A:358:GLY:O	2.11	0.49
1:B:228:VAL:HA	1:B:266:THR:CG2	2.43	0.49
1:B:283:HIS:O	1:B:286:ALA:HB3	2.12	0.49
1:B:65:LEU:HD13	1:B:100:TYR:HB2	1.95	0.48
1:B:203:ILE:O	1:B:207:ILE:HG13	2.13	0.48
1:B:209:VAL:HA	1:B:215:THR:CG2	2.43	0.48
1:A:139:PRO:HA	1:A:142:LYS:HE2	1.94	0.48
1:B:114:GLU:OE2	1:B:118:ARG:HD3	2.13	0.48
1:A:198:ARG:HG3	1:A:198:ARG:HH11	1.78	0.48
1:B:372:ASN:ND2	1:B:405:PHE:N	2.53	0.48
1:A:351:LYS:HA	1:A:356:GLU:O	2.14	0.48
1:B:323:VAL:H	1:B:326:GLN:HE21	1.60	0.48
1:A:42:ILE:HG22	1:A:45:TRP:H	1.79	0.47
1:A:198:ARG:HH22	1:A:233:THR:HG21	1.80	0.47
1:A:260:ARG:HE	1:A:264:GLN:HE21	1.61	0.47
1:A:364:LYS:NZ	1:A:364:LYS:HB3	2.29	0.47
1:B:196:LEU:HD13	1:B:200:GLU:HB2	1.96	0.47
1:B:367:ASP:HB3	1:B:370:SER:CB	2.43	0.47
1:B:222:GLU:O	1:B:226:LYS:HB3	2.14	0.47
1:B:169:ILE:HD11	1:B:254:TRP:HH2	1.80	0.47
1:B:117:ASP:HB2	1:B:177:ASN:CG	2.40	0.46
1:A:95:HIS:HD2	1:A:95:HIS:O	1.97	0.46
1:A:429:ILE:HD12	1:A:429:ILE:N	2.30	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:THR:HG22	1:A:140:VAL:HG12	1.98	0.46
1:B:371:TYR:HE2	1:B:421:ILE:O	1.98	0.46
1:B:268:MSE:CE	1:B:269:LEU:HG	2.37	0.46
1:B:421:ILE:HD11	1:B:426:ALA:CB	2.46	0.46
1:A:180:VAL:HG13	1:A:258:ASN:HD22	1.80	0.46
1:B:127:LEU:HD11	1:B:167:ARG:HE	1.80	0.46
1:B:159:ASN:HB3	1:B:162:HIS:ND1	2.30	0.46
1:B:233:THR:HA	1:B:236:ALA:CB	2.43	0.46
1:B:371:TYR:CE2	1:B:402:HIS:HB2	2.50	0.46
1:B:225:GLU:OE2	1:B:229:LEU:HB2	2.16	0.46
1:A:117:ASP:O	1:A:120:LEU:HB2	2.15	0.46
1:A:42:ILE:HD12	1:A:42:ILE:N	2.31	0.46
1:A:119:ALA:HA	1:A:122:LEU:HB2	1.97	0.45
1:B:194:LYS:H	1:B:194:LYS:CD	2.18	0.45
1:B:339:ILE:HG12	1:B:429:ILE:HB	1.98	0.45
1:B:174:GLN:O	1:B:213:MSE:HG3	2.17	0.45
1:B:92:THR:O	1:B:95:HIS:HB3	2.16	0.45
1:B:316:LEU:O	1:B:320:TYR:HB2	2.17	0.45
1:A:167:ARG:HG3	1:A:167:ARG:HH11	1.82	0.45
1:B:51:LYS:HG3	1:B:71:MSE:HE1	1.99	0.45
1:A:185:ILE:HD11	1:A:203:ILE:HG12	1.98	0.45
1:A:203:ILE:O	1:A:207:ILE:HG13	2.17	0.45
1:A:342:SER:HB3	1:A:432:GLN:HE22	1.82	0.45
1:B:306:HIS:ND1	1:B:307:ASN:N	2.65	0.45
1:B:384:PHE:HB3	1:B:431:VAL:HG22	1.99	0.45
1:B:41:GLN:HE22	1:B:42:ILE:HG12	1.78	0.45
1:B:179:ASN:HD22	1:B:179:ASN:HA	1.59	0.44
1:B:221:LYS:HD3	1:B:224:LYS:HD3	1.99	0.44
1:A:112:LEU:H	1:A:112:LEU:HD23	1.82	0.44
1:A:225:GLU:O	1:A:226:LYS:C	2.61	0.44
1:B:45:TRP:O	1:B:49:HIS:HB2	2.17	0.44
1:B:322:LYS:HD3	1:B:327:HIS:CE1	2.52	0.44
1:B:204:LYS:HA	1:B:207:ILE:HD12	2.00	0.44
1:B:209:VAL:HA	1:B:215:THR:HG21	1.99	0.44
1:B:377:GLN:HE21	1:B:377:GLN:HA	1.82	0.44
1:A:135:GLN:HE21	1:A:135:GLN:HB3	1.69	0.44
1:B:254:TRP:CE3	1:B:293:TRP:HH2	2.36	0.44
1:B:184:ILE:O	1:B:188:ILE:HG12	2.18	0.44
1:B:345:GLU:CA	1:B:363:LEU:HD23	2.48	0.44
1:A:429:ILE:HG22	1:A:430:LEU:N	2.32	0.44
1:B:61:SER:O	1:B:62:LEU:HB2	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:ARG:HH11	1:B:167:ARG:HG3	1.83	0.44
1:B:190:ALA:O	1:B:191:ASN:ND2	2.51	0.44
1:A:60:ALA:O	1:A:61:SER:C	2.61	0.44
1:A:223:GLU:HG3	1:A:224:LYS:N	2.32	0.43
1:B:257:GLN:O	1:B:261:ILE:HG12	2.17	0.43
1:B:377:GLN:HA	1:B:377:GLN:NE2	2.34	0.43
1:A:268:MSE:HE3	1:A:269:LEU:HD11	2.00	0.43
1:B:196:LEU:HD13	1:B:196:LEU:C	2.42	0.43
1:A:350:VAL:HG22	1:A:351:LYS:N	2.33	0.43
1:A:188:ILE:O	1:A:188:ILE:HG22	2.19	0.43
1:A:236:ALA:O	1:A:239:GLU:HB3	2.18	0.43
1:B:111:VAL:HA	1:B:169:ILE:O	2.19	0.43
1:B:82:GLU:OE2	1:B:85:HIS:ND1	2.52	0.43
1:B:213:MSE:O	1:B:217:GLU:HB2	2.19	0.43
1:B:242:LYS:HG2	1:B:247:GLY:HA3	2.01	0.43
1:A:271:THR:HB	1:A:272:PRO:CD	2.48	0.42
1:B:333:GLY:C	1:B:335:ARG:H	2.27	0.42
1:A:368:PRO:HA	1:A:373:TYR:CD2	2.54	0.42
1:A:372:ASN:ND2	1:A:404:ILE:HA	2.34	0.42
1:B:271:THR:HB	1:B:272:PRO:HD3	2.02	0.42
1:A:192:ASN:O	1:A:194:LYS:N	2.52	0.42
1:B:174:GLN:HB3	1:B:213:MSE:HE2	2.01	0.42
1:A:264:GLN:HG2	2:A:464:HOH:O	2.19	0.42
1:B:69:LYS:HG2	1:B:105:LYS:HD3	2.02	0.42
1:B:187:TYR:CD2	1:B:255:ILE:HG13	2.54	0.42
1:B:347:GLN:HB3	1:B:438:PRO:HG3	2.02	0.42
1:A:278:ASP:O	1:A:282:LYS:HG3	2.18	0.42
1:B:331:TYR:CD1	1:B:331:TYR:C	2.97	0.42
1:A:42:ILE:HG23	1:A:44:LYS:HB3	2.00	0.42
1:A:66:LYS:N	1:A:67:PRO:CD	2.82	0.42
1:A:54:LYS:HE2	1:A:55:THR:CG2	2.48	0.42
1:A:254:TRP:HE3	1:A:293:TRP:HH2	1.68	0.42
1:A:338:SER:OG	1:A:427:PHE:HA	2.19	0.42
1:A:423:LEU:HD21	1:A:430:LEU:CD1	2.41	0.42
1:B:188:ILE:HG22	1:B:245:LEU:HD22	2.02	0.42
1:B:42:ILE:O	1:B:42:ILE:HG22	2.20	0.42
1:A:41:GLN:HB3	1:A:42:ILE:CD1	2.47	0.42
1:A:98:VAL:O	1:A:102:VAL:HG23	2.20	0.42
1:A:198:ARG:HH22	1:A:233:THR:CG2	2.32	0.42
1:B:143:THR:HB	1:B:145:GLU:OE1	2.20	0.42
1:A:281:LEU:O	1:A:285:ILE:HG13	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:GLU:HA	1:B:363:LEU:HB3	2.02	0.41
1:B:352:ASN:HD21	1:B:356:GLU:HB2	1.85	0.41
1:A:89:GLU:H	1:A:89:GLU:CD	2.27	0.41
1:A:99:LYS:HG3	1:A:152:TRP:CZ2	2.55	0.41
1:A:225:GLU:HB3	1:A:226:LYS:H	1.49	0.41
1:A:322:LYS:HD3	1:A:327:HIS:CE1	2.55	0.41
1:B:119:ALA:HA	1:B:122:LEU:HD12	2.01	0.41
1:B:272:PRO:HG2	1:B:279:PHE:HB2	2.02	0.41
1:A:381:ASP:HB3	1:A:382:GLN:NE2	2.35	0.41
1:B:203:ILE:HD12	1:B:203:ILE:C	2.45	0.41
1:B:65:LEU:O	1:B:68:LEU:HB2	2.20	0.41
1:B:207:ILE:N	1:B:208:PRO:HD2	2.35	0.41
1:B:227:TYR:HA	1:B:230:ASP:HB2	2.02	0.41
1:A:237:LEU:C	1:A:237:LEU:HD23	2.46	0.41
1:B:81:GLY:HA2	1:B:305:GLY:O	2.21	0.41
1:A:117:ASP:HB2	1:A:177:ASN:CG	2.45	0.41
1:A:292:LYS:O	1:A:296:GLU:HG3	2.21	0.41
1:A:428:ASP:C	1:A:429:ILE:HD12	2.45	0.41
1:B:57:ASN:HA	1:B:58:PRO:HD3	1.93	0.41
1:B:77:ILE:HG23	1:B:336:TYR:CD1	2.54	0.41
1:A:40:ASN:O	1:A:41:GLN:C	2.64	0.41
1:A:58:PRO:HD3	1:A:92:THR:HB	2.03	0.41
1:A:82:GLU:OE2	1:A:85:HIS:CD2	2.69	0.41
1:A:398:LEU:HD12	1:A:398:LEU:HA	1.95	0.41
1:A:99:LYS:HG3	1:A:152:TRP:CE2	2.56	0.41
1:B:42:ILE:HG13	1:B:393:VAL:CG1	2.51	0.40
1:B:159:ASN:HA	1:B:160:PRO:HD3	1.94	0.40
1:B:123:ASP:O	1:B:126:VAL:HG22	2.21	0.40
1:B:221:LYS:HA	1:B:221:LYS:CE	2.51	0.40
1:A:307:ASN:HD22	1:A:307:ASN:HA	1.62	0.40
1:A:315:MSE:HG3	1:A:316:LEU:CD1	2.51	0.40
1:A:45:TRP:CH2	1:A:390:ALA:HB2	2.56	0.40
1:A:87:ALA:HB3	1:A:90:VAL:CG2	2.52	0.40
1:A:406:ALA:HB2	1:A:419:VAL:HG13	2.02	0.40
1:A:428:ASP:CB	1:A:429:ILE:HD12	2.51	0.40
1:B:46:LEU:HD12	1:B:385:ILE:HD13	2.04	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	401/451 (89%)	350 (87%)	39 (10%)	12 (3%)	3	6
1	B	403/451 (89%)	355 (88%)	40 (10%)	8 (2%)	6	11
All	All	804/902 (89%)	705 (88%)	79 (10%)	20 (2%)	4	8

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	271	THR
1	A	273	PRO
1	B	220	THR
1	B	249	SER
1	B	273	PRO
1	A	41	GLN
1	A	194	LYS
1	A	247	GLY
1	B	54	LYS
1	A	193	SER
1	A	220	THR
1	A	248	LYS
1	B	352	ASN
1	A	61	SER
1	B	224	LYS
1	A	189	LYS
1	A	226	LYS
1	A	434	GLN
1	B	225	GLU
1	B	173	ILE

5.3.2 Protein sidechains [i](#)

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	354/386 (92%)	333 (94%)	21 (6%)	18	33
1	B	356/386 (92%)	338 (95%)	18 (5%)	21	40
All	All	710/772 (92%)	671 (94%)	39 (6%)	19	37

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	LEU
1	A	63	ASN
1	A	64	ASP
1	A	112	LEU
1	A	161	LYS
1	A	164	SER
1	A	220	THR
1	A	221	LYS
1	A	225	GLU
1	A	235	SER
1	A	240	GLU
1	A	260	ARG
1	A	266	THR
1	A	284	ASP
1	A	307	ASN
1	A	319	ILE
1	A	363	LEU
1	A	369	ASN
1	A	396	THR
1	A	398	LEU
1	A	409	THR
1	B	53	LEU
1	B	63	ASN
1	B	139	PRO
1	B	155	GLN
1	B	179	ASN
1	B	192	ASN
1	B	194	LYS
1	B	201	GLU
1	B	204	LYS
1	B	221	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	232	LYS
1	B	237	LEU
1	B	316	LEU
1	B	398	LEU
1	B	409	THR
1	B	410	THR
1	B	422	SER
1	B	436	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	HIS
1	A	63	ASN
1	A	85	HIS
1	A	88	HIS
1	A	95	HIS
1	A	109	ASN
1	A	135	GLN
1	A	136	HIS
1	A	155	GLN
1	A	157	ASN
1	A	174	GLN
1	A	179	ASN
1	A	214	ASN
1	A	257	GLN
1	A	258	ASN
1	A	290	ASN
1	A	307	ASN
1	A	314	ASN
1	A	326	GLN
1	A	372	ASN
1	A	399	ASN
1	A	401	GLN
1	A	402	HIS
1	A	432	GLN
1	A	434	GLN
1	B	109	ASN
1	B	136	HIS
1	B	155	GLN
1	B	157	ASN
1	B	174	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	179	ASN
1	B	182	ASN
1	B	183	ASN
1	B	191	ASN
1	B	192	ASN
1	B	241	ASN
1	B	246	ASN
1	B	257	GLN
1	B	258	ASN
1	B	290	ASN
1	B	307	ASN
1	B	314	ASN
1	B	326	GLN
1	B	327	HIS
1	B	349	ASN
1	B	372	ASN
1	B	377	GLN
1	B	432	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [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 ⓘ

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	395/451 (87%)	-0.04	10 (2%) 58 56	33, 56, 90, 103	0
1	B	397/451 (88%)	0.01	2 (0%) 87 87	33, 64, 91, 104	0
All	All	792/902 (87%)	-0.02	12 (1%) 72 71	33, 61, 91, 104	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	270	ALA	4.0
1	A	271	THR	2.9
1	A	61	SER	2.8
1	A	223	GLU	2.7
1	A	42	ILE	2.5
1	A	392	GLY	2.5
1	B	271	THR	2.3
1	B	343	VAL	2.3
1	A	225	GLU	2.2
1	A	442	HIS	2.1
1	A	43	ALA	2.1
1	A	46	LEU	2.1

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.