



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 07:46 am GMT

PDB ID : 2RAD
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

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

with specific help available everywhere you see the ⓘ symbol.

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

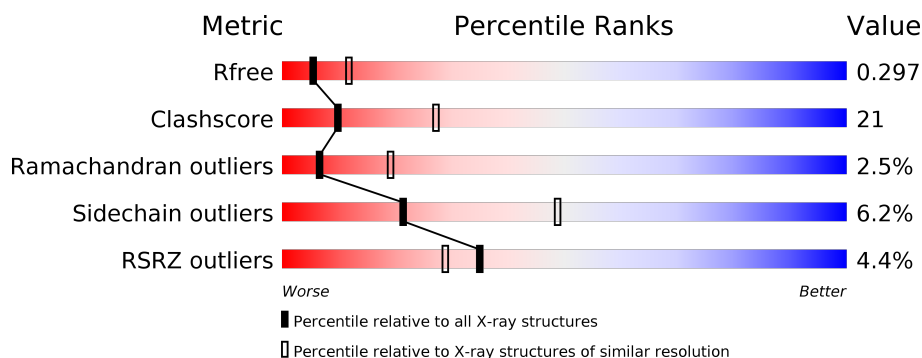
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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}	100719	3666 (2.80-2.72)
Clashscore	112137	4174 (2.80-2.72)
Ramachandran outliers	110173	4103 (2.80-2.72)
Sidechain outliers	110143	4106 (2.80-2.72)
RSRZ outliers	101464	3697 (2.80-2.72)

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 $\leq 5\%$. 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	<div> <div>5%</div> <div> <div></div> <div>52%</div> <div>33%</div> <div>•</div> <div>11%</div> </div> </div>
1	B	451	<div> <div>2%</div> <div> <div></div> <div>46%</div> <div>41%</div> <div>•</div> <div>10%</div> </div> </div>

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.

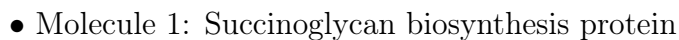
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	21	Total	O	0	0
			21	21		

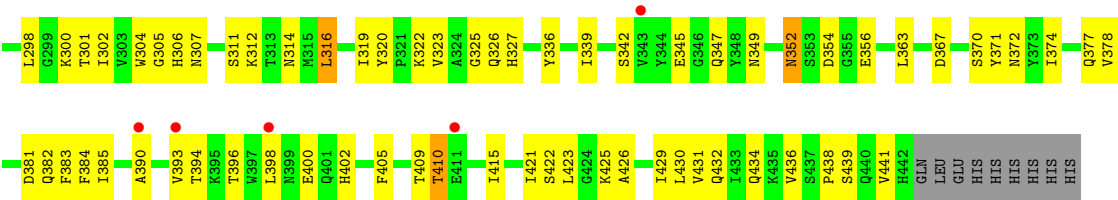
Continued on next page...

Continued from previous page...

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

- 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 46.01 – 2.75	Depositor EDS
% Data completeness (in resolution range)	82.1 (19.93-2.75) 94.9 (46.01-2.75)	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 0.224 , 0.297	Depositor DCC
R_{free} test set	2171 reflections (9.77%)	DCC
Wilson B-factor (Å ²)	50.6	Xtriage
Anisotropy	0.726	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 44.5	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	0.92	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 [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	0.44	0/3298	0.67	1/4450 (0.0%)
1	B	0.40	0/3313	0.63	1/4471 (0.0%)
All	All	0.42	0/6611	0.65	2/8921 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	112	LEU	CA-CB-CG	5.33	127.55	115.30
1	B	43	ALA	N-CA-C	-5.02	97.44	111.00

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	131	0
1	B	3245	0	3252	145	0
2	A	21	0	0	1	0
2	B	10	0	0	0	0
All	All	6506	0	6491	276	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 21.

All (276) 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
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:H	1:B:374:ILE:HD12	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:B:221:LYS:HA	1:B:221:LYS:NZ	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:LYS:HD3	1:B:194:LYS:H	1.61	0.65
1:A:372:ASN:HD21	1:A:405:PHE:N	1.91	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
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:80:LEU:HG	1:A:94:LYS:HE3	1.81	0.63
1:B:132:ASN:ND2	1:B:135:GLN:HG2	2.14	0.62
1:A:138:THR:HG23	1:A:139:PRO:HD2	1.81	0.62
1:A:83:ALA:O	1:A:407:GLY:HA3	1.99	0.62
1:A:45:TRP:CZ3	1:A:385:ILE:HD11	2.34	0.62
1:B:221:LYS:HA	1:B:221:LYS:HZ1	1.64	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:B:319:ILE:HG13	1:B:320:TYR:N	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: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: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:HD13	1:B:196:LEU:O	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: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

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:432:GLN:C	1:A:433:ILE:HD12	2.27	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:107:PHE:CD2	1:B:300:LYS:HB3	2.43	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:NZ	1:B:204:LYS:HB2	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:236:ALA:O	1:B:240:GLU:HG2	2.10	0.52
1:B:81:GLY:HA3	1:B:307:ASN:HD22	1.74	0.52
1:B:410:THR:HG23	1:B:415:ILE:HD13	1.90	0.52
1:B:294:THR:HG23	1:B:298:LEU:HD12	1.91	0.52
1:B:61:SER:OG	1:B:63:ASN:HB2	2.09	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:B:41:GLN:CD	1:B:42:ILE:HG12	2.31	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:137:LEU:HD21	1:B:146:MSE:HE2	1.92	0.51
1:B:77:ILE:HG23	1:B:336:TYR:HD1	1.75	0.51
1:B:86:GLY:C	1:B:439:SER:HB2	2.31	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: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:N	1:A:433:ILE:HD12	2.27	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: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: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:A:195:LEU:HD11	1:A:241:ASN:CG	2.33	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:HH11	1:A:198:ARG:HG3	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:364:LYS:NZ	1:A:364:LYS:HB3	2.29	0.47
1:A:260:ARG:HE	1:A:264:GLN:HE21	1.61	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:A:429:ILE:HD12	1:A:429:ILE:N	2.30	0.46
1:A:95:HIS:HD2	1:A:95:HIS:O	1.97	0.46
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:138:THR:O	1:A:139:PRO:C	2.54	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:N	1:A:42:ILE:HD12	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:A:272:PRO:HD3	1:A:282:LYS:HZ3	1.81	0.45
1:B:316:LEU:O	1:B:320:TYR:HB2	2.17	0.45
1:B:92:THR:O	1:B:95:HIS:HB3	2.16	0.45
1:A:167:ARG:HG3	1:A:167:ARG:HH11	1.82	0.45
1:A:95:HIS:CD2	1:A:95:HIS:C	2.90	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:39:THR:C	1:B:41:GLN:H	2.20	0.45
1:B:240:GLU:C	1:B:242:LYS:H	2.20	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:HA	1:B:179:ASN:HD22	1.59	0.44
1:B:221:LYS:HD3	1:B:224:LYS:HD3	1.99	0.44
1:A:112:LEU:HD23	1:A:112:LEU:H	1.82	0.44
1:B:322:LYS:HD3	1:B:327:HIS:CE1	2.52	0.44
1:B:45:TRP:O	1:B:49:HIS:HB2	2.17	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:HA	1:B:377:GLN:HE21	1.82	0.44
1:A:135:GLN:HE21	1:A:135:GLN:HB3	1.69	0.44
1:A:429:ILE:HG22	1:A:430:LEU:N	2.32	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:ARG:HG3	1:B:167:ARG:HH11	1.83	0.44
1:B:190:ALA:O	1:B:191:ASN:ND2	2.51	0.44
1:B:61:SER:O	1:B:62:LEU:HB2	2.18	0.44
1:A:223:GLU:HG3	1:A:224:LYS:N	2.32	0.43
1:A:272:PRO:HD3	1:A:282:LYS:HZ1	1.83	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:204:LYS:HZ2	1:B:204:LYS:HB2	1.84	0.43
1:A:350:VAL:HG22	1:A:351:LYS:N	2.33	0.43
1:A:188:ILE:HG22	1:A:188:ILE:O	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: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:B:82:GLU:OE2	1:B:85:HIS:ND1	2.52	0.43
1:A:271:THR:HB	1:A:272:PRO:CD	2.48	0.42
1:A:372:ASN:ND2	1:A:404:ILE:HA	2.34	0.42
1:A:368:PRO:HA	1:A:373:TYR:CD2	2.54	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:117:ASP:HB2	1:B:177:ASN:CG	2.40	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: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:B:42:ILE:O	1:B:42:ILE:HG22	2.20	0.42
1:B:69:LYS:HG2	1:B:105:LYS:HD3	2.02	0.42
1:A:278:ASP:O	1:A:282:LYS:HG3	2.18	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: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:A:54:LYS:HE2	1:A:55:THR:CG2	2.48	0.42
1:B:188:ILE:HG22	1:B:245:LEU:HD22	2.02	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:A:41:GLN:HB3	1:A:42:ILE:CD1	2.47	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: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:A:99:LYS:HG3	1:A:152:TRP:CZ2	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: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:B:81:GLY:HA2	1:B:305:GLY:O	2.21	0.41
1:A:292:LYS:O	1:A:296:GLU:HG3	2.21	0.41
1:B:77:ILE:HG23	1:B:336:TYR:CD1	2.54	0.41
1:B:57:ASN:HA	1:B:58:PRO:HD3	1.93	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:58:PRO:HD3	1:A:92:THR:HB	2.03	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:CE	1:B:221:LYS:HA	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: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:A:87:ALA:HB3	1:A:90:VAL:CG2	2.52	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 ⓘ

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	401/451 (89%)	350 (87%)	39 (10%)	12 (3%)	5	15
1	B	403/451 (89%)	355 (88%)	40 (10%)	8 (2%)	9	25
All	All	804/902 (89%)	705 (88%)	79 (10%)	20 (2%)	6	19

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 ⓘ

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%)	330 (93%)	24 (7%)	18	43

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	356/386 (92%)	336 (94%)	20 (6%)	25	53
All	All	710/772 (92%)	666 (94%)	44 (6%)	21	49

All (44) 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	246	ASN
1	A	260	ARG
1	A	266	THR
1	A	281	LEU
1	A	284	ASP
1	A	307	ASN
1	A	314	ASN
1	A	319	ILE
1	A	363	LEU
1	A	369	ASN
1	A	396	THR
1	A	409	THR
1	A	430	LEU
1	B	53	LEU
1	B	63	ASN
1	B	118	ARG
1	B	155	GLN
1	B	179	ASN
1	B	192	ASN
1	B	194	LYS
1	B	201	GLU
1	B	211	LYS
1	B	221	LYS
1	B	230	ASP
1	B	260	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	314	ASN
1	B	316	LEU
1	B	354	ASP
1	B	398	LEU
1	B	409	THR
1	B	410	THR
1	B	422	SER
1	B	436	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	85	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	192	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	382	GLN
1	A	399	ASN
1	A	401	GLN
1	A	432	GLN
1	B	109	ASN
1	B	132	ASN
1	B	136	HIS
1	B	155	GLN
1	B	157	ASN
1	B	179	ASN
1	B	182	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.27	24 (6%) 22 17	33, 56, 90, 103	0
1	B	397/451 (88%)	0.18	11 (2%) 53 48	33, 64, 91, 104	0
All	All	792/902 (87%)	0.22	35 (4%) 35 29	33, 61, 91, 104	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	391	ASN	4.9
1	A	199	VAL	4.3
1	A	244	TYR	4.0
1	A	392	GLY	4.0
1	A	275	LYS	3.7
1	B	393	VAL	3.6
1	A	243	SER	3.4
1	B	398	LEU	3.4
1	A	270	ALA	3.1
1	A	203	ILE	2.9
1	B	38	ASN	2.8
1	B	46	LEU	2.7
1	A	196	LEU	2.7
1	A	40	ASN	2.6
1	A	271	THR	2.6
1	A	395	LYS	2.6
1	A	394	THR	2.5
1	A	200	GLU	2.5
1	A	197	PRO	2.4
1	A	393	VAL	2.4
1	A	234	ILE	2.3
1	B	343	VAL	2.3
1	A	61	SER	2.3
1	A	223	GLU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	271	THR	2.3
1	A	66	LYS	2.3
1	B	265	PHE	2.3
1	B	250	LYS	2.2
1	A	274	ASP	2.2
1	B	280	TYR	2.2
1	A	216	PHE	2.1
1	B	390	ALA	2.1
1	A	46	LEU	2.1
1	A	242	LYS	2.1
1	B	411	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.