Full wwPDB X-ray Structure Validation Report (i)

Jun 15, 2024 – 11:51 AM EDT

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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

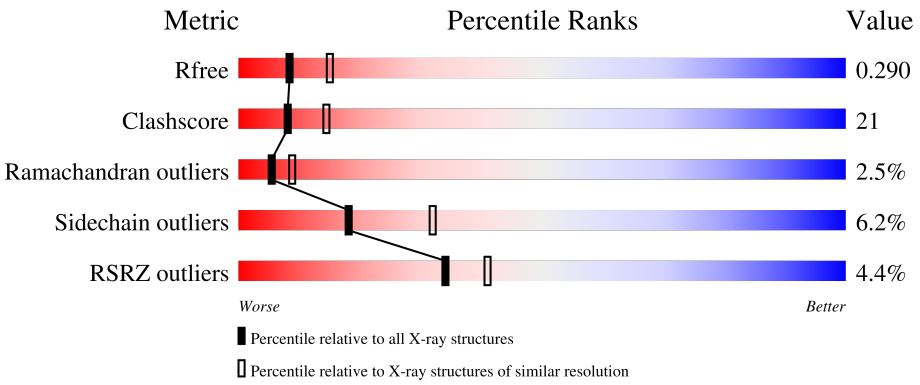
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

1 Overall quality at a glance (i)

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}	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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 <=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	5% 52% 33% • 11%
1	B	451	2% 46% 41% • 10%

Validation Pipeline (wwPDB-VP) : 2.37.1

2 Entry composition (i)

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
			Total	C	N	O	Se			
1	A	403	3230	2071	547	604	8	0	0	0
1	B	405	3245	2079	550	608	8	0	0	0

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
			Total	O		
2	A	21	21	21	0	0

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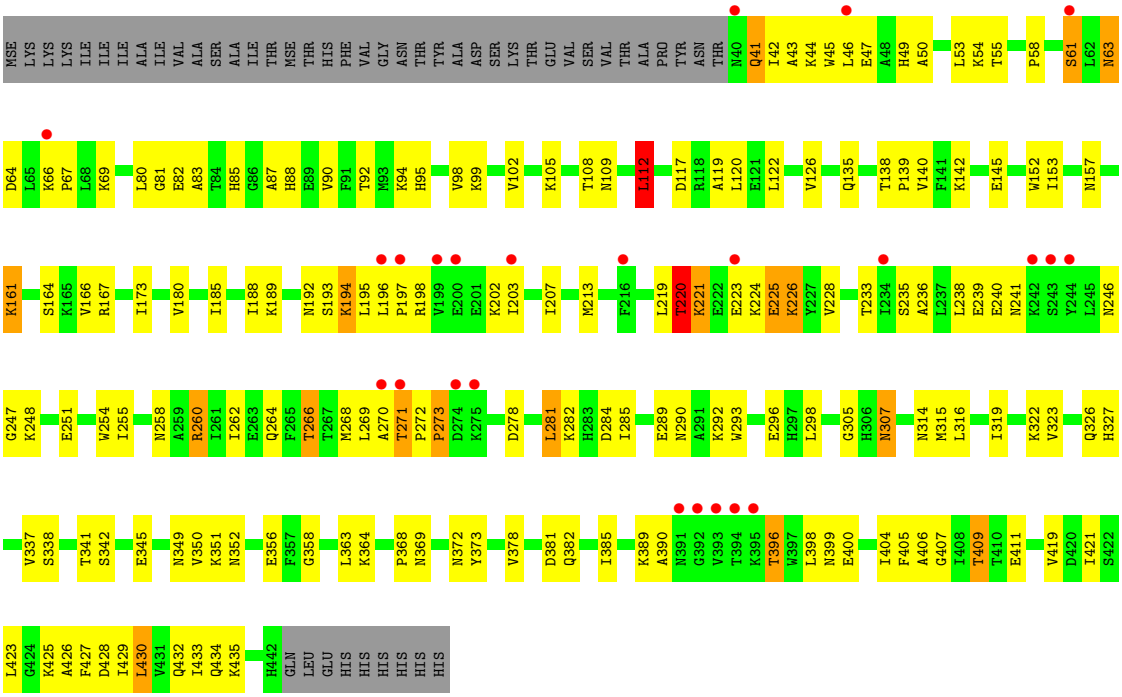
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	B	10	10	10	0	0

3 Residue-property plots (i)

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.

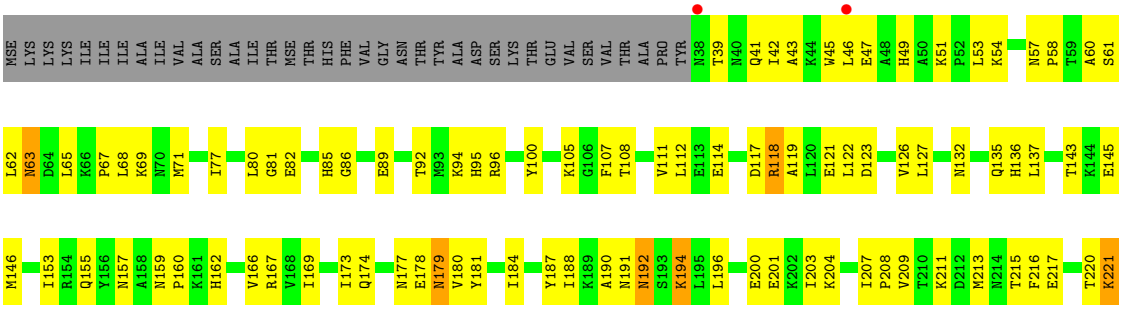
• Molecule 1: Succinoglycan biosynthesis protein

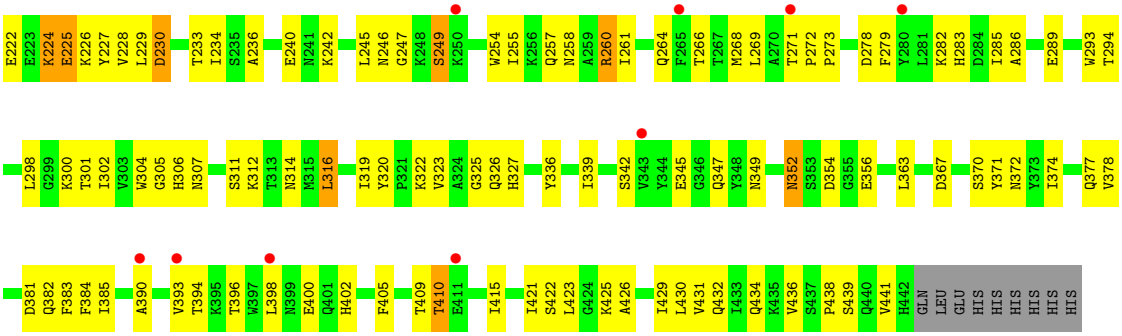
Chain A:



• Molecule 1: Succinoglycan biosynthesis protein

Chain B:




E222 E223 K224 E225 K226 Y227 V228 L229 D230
T233 I234 S235 A236
E240 N241 K242
L245 N246 G247 K248 S249 K250
W254 I255 K256 Q257 N258 A259 R260 I261
Q264 F265 T266 T267 M268 L269 A270 T271 P272 P273
D278 F279 Y280 L281 K282 H283 D284 I285 A286
E289
W293 T294
L298 G299 K300 T301 I302 V303 W304 G305 H306 N307
S311 K312 T313 N314 M315 L316
I319 Y320 P321 K322 V323 A324 G325 Q326 H327
Y336
I339
S342 V343 Y344 E345 G346 Q347 Y348 N349
N352 S353 D354 G355 E356
L363
D367
S370 Y371 N372 Y373 I374
Q377 V378
D381 Q382 F383 F384 I385
A390
V393 T394 K395 T396 W397 L398 N399 E400 Q401 H402
F405
T409 T410 E411
I415
I421 S422 L423 G424 K425 A426
I429 L430 V431 Q432 I433 Q434 K435 V436 S437 P438 S439 Q440 V441 H442
GLN LEU GLU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	2.35 (at 2.77Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.209 , 0.281 0.218 , 0.290	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)	0.31 , 44.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[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 (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(^{o})	Ideal(^{o})
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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: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: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

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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: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: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: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: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: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

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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: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: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: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
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

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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: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:A:272:PRO:HD3	1:A:282:LYS:HZ3	1.81	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:95:HIS:C	1:A:95:HIS:CD2	2.90	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: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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:SER:O	1:B:62:LEU:HB2	2.18	0.44
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: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:HB2	1:B:204:LYS:HZ2	1.84	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: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: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:42:ILE:HG22	1:B:42:ILE:O	2.20	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: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: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

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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: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: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: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: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%)	4 6
1	B	403/451 (89%)	355 (88%)	40 (10%)	8 (2%)	7 13
All	All	804/902 (89%)	705 (88%)	79 (10%)	20 (2%)	5 9

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%)	330 (93%)	24 (7%)	16 28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	356/386 (92%)	336 (94%)	20 (6%)	21	36
All	All	710/772 (92%)	666 (94%)	44 (6%)	18	32

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

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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

Sometimes 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

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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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	395/451 (87%)	0.27	24 (6%)	21	26	33, 56, 90, 103	0
1	B	397/451 (88%)	0.18	11 (2%)	53	62	33, 64, 91, 104	0
All	All	792/902 (87%)	0.22	35 (4%)	34	41	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	A	61	SER	2.3
1	B	343	VAL	2.3
1	A	223	GLU	2.3

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