



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:15 AM UTC

PDB ID : 7MZT / pdb_00007mzt
Title : Borrelia burgdorferi BBK32-C in complex with an autolytic fragment of human C1r at 4.1Å
Authors : Garcia, B.L.
Deposited on : 2021-05-24
Resolution : 4.07 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
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)
Validation Pipeline (wwPDB-VP) : 2.49

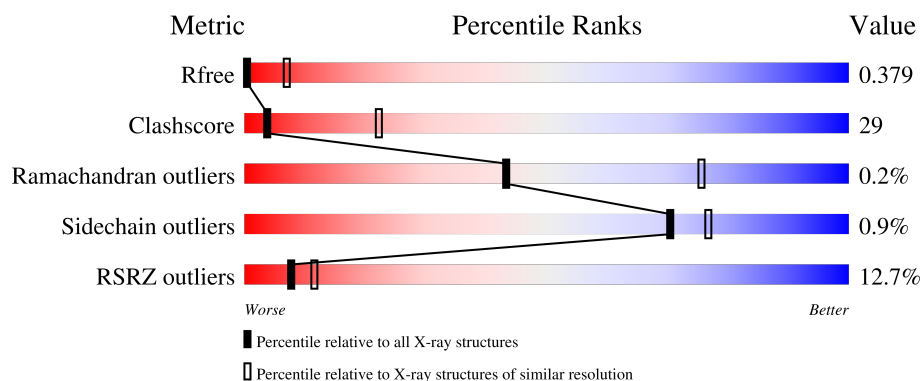
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.07 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	1200 (4.36-3.80)
Clashscore	190562	1249 (4.36-3.80)
Ramachandran outliers	187476	1169 (4.36-3.80)
Sidechain outliers	187428	1158 (4.36-3.80)
RSRZ outliers	180081	1199 (4.36-3.80)

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	164	
2	B	242	
3	I	148	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4120 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 Complement C1r subcomponent heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	142	Total	C	N	O	S	0	0	0
			1153	728	202	211	12			

- Molecule 2 is a protein called Complement C1r subcomponent light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	233	Total	C	N	O	S	0	0	0
			1835	1166	320	337	12			

- Molecule 3 is a protein called Fibronectin-binding protein BBK32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	138	Total	C	N	O	S	0	0	0
			1118	719	182	215	2			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	201	GLY	-	expression tag	UNP O50835
I	202	SER	-	expression tag	UNP O50835
I	203	THR	-	expression tag	UNP O50835
I	204	GLY	-	expression tag	UNP O50835
I	205	SER	-	expression tag	UNP O50835

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

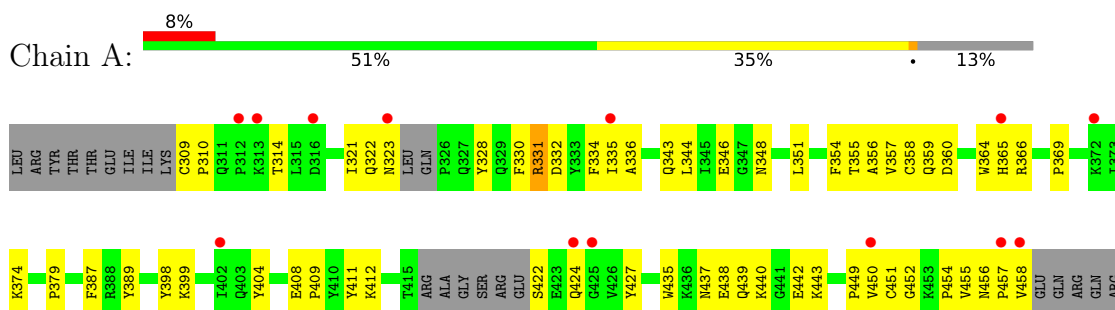


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	B	1	14	8	1	5	0	0

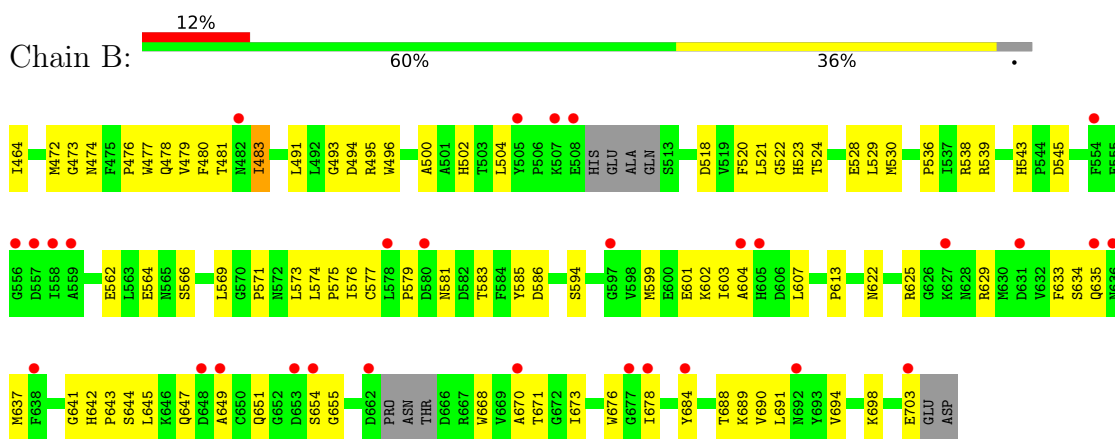
3 Residue-property plots

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.

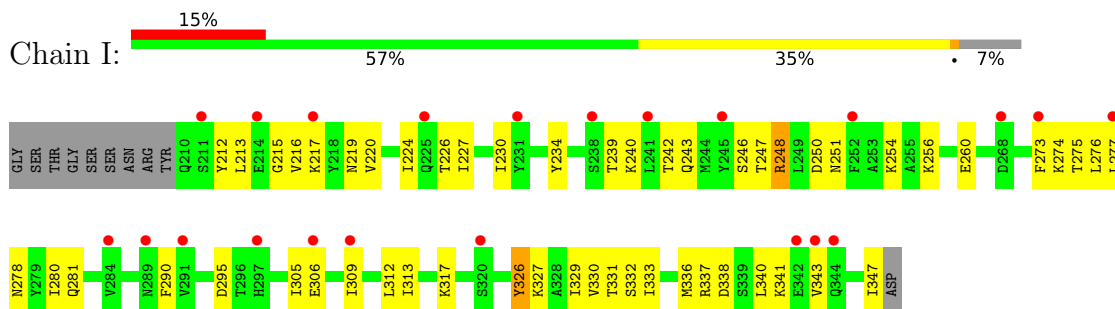
- Molecule 1: Complement C1r subcomponent heavy chain



- Molecule 2: Complement C1r subcomponent light chain



- Molecule 3: Fibronectin-binding protein BBK32



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	113.62Å 96.99Å 108.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.26 – 4.07 44.26 – 4.07	Depositor EDS
% Data completeness (in resolution range)	83.8 (44.26-4.07) 75.0 (44.26-4.07)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	-0.53 (at 4.00Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.369 , 0.372 0.370 , 0.379	Depositor DCC
R_{free} test set	854 reflections (10.06%)	wwPDB-VP
Wilson B-factor (Å ²)	89.1	Xtriage
Anisotropy	1.151	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 94.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.017 for l,-k,h	Xtriage
F_o, F_c correlation	0.71	EDS
Total number of atoms	4120	wwPDB-VP
Average B, all atoms (Å ²)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.51 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.1310e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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	0.59	0/1183	0.89	0/1600
2	B	0.46	0/1880	0.84	1/2543 (0.0%)
3	I	0.65	0/1132	0.97	0/1523
All	All	0.56	0/4195	0.89	1/5666 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	483	ILE	N-CA-C	5.05	119.84	109.34

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	1153	0	1104	83	0
2	B	1835	0	1763	119	0
3	I	1118	0	1162	84	0
4	B	14	0	13	0	0
All	All	4120	0	4042	235	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 29.

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)
3:I:213:LEU:HA	3:I:216:VAL:HG12	1.27	1.16
2:B:518:ASP:CG	3:I:327:LYS:HE3	1.72	1.13
2:B:673:ILE:CG2	2:B:688:THR:HB	1.86	1.04
1:A:346:GLU:OE2	1:A:366:ARG:HG2	1.59	1.00
2:B:518:ASP:CG	3:I:327:LYS:CE	2.40	0.95
1:A:455:VAL:HG21	2:B:571:PRO:HB3	1.50	0.93
3:I:281:GLN:HG3	3:I:306:GLU:OE2	1.70	0.92
3:I:327:LYS:O	3:I:330:VAL:HG12	1.69	0.92
3:I:213:LEU:CD2	3:I:290:PHE:HZ	1.84	0.90
3:I:290:PHE:CD2	3:I:295:ASP:HB3	2.07	0.90
3:I:213:LEU:HA	3:I:216:VAL:CG1	2.02	0.90
2:B:603:ILE:HG12	3:I:239:THR:OG1	1.73	0.89
1:A:455:VAL:HG21	2:B:571:PRO:CB	2.04	0.87
1:A:346:GLU:OE2	1:A:366:ARG:CG	2.21	0.86
2:B:673:ILE:HG23	2:B:688:THR:HB	1.56	0.86
3:I:277:LEU:HB2	3:I:309:ILE:HG21	1.56	0.86
2:B:518:ASP:OD2	3:I:327:LYS:HE3	1.75	0.86
1:A:457:PRO:O	1:A:458:VAL:HG23	1.76	0.85
1:A:346:GLU:HB2	1:A:369:PRO:HB3	1.58	0.85
2:B:518:ASP:CB	3:I:327:LYS:HE3	2.08	0.83
1:A:454:PRO:CG	1:A:457:PRO:HB3	2.09	0.82
2:B:673:ILE:HG22	2:B:688:THR:O	1.79	0.82
1:A:454:PRO:HG2	1:A:457:PRO:CB	2.10	0.81
1:A:331:ARG:CB	1:A:331:ARG:HH11	1.95	0.78
3:I:213:LEU:HD21	3:I:290:PHE:HZ	1.49	0.78
3:I:290:PHE:CG	3:I:295:ASP:HB3	2.19	0.77
1:A:454:PRO:HG2	1:A:457:PRO:HB3	1.64	0.77
1:A:454:PRO:O	1:A:457:PRO:HD3	1.83	0.77
2:B:649:ALA:HB3	3:I:248:ARG:NH2	2.01	0.76
2:B:649:ALA:HB3	3:I:248:ARG:HH22	1.51	0.75
2:B:483:ILE:HD13	2:B:504:LEU:HD23	1.69	0.74
3:I:213:LEU:HD21	3:I:290:PHE:CZ	2.21	0.74
2:B:518:ASP:CG	3:I:327:LYS:NZ	2.45	0.74
3:I:213:LEU:CA	3:I:216:VAL:HG12	2.14	0.74
1:A:322:GLN:O	1:A:323:ASN:OD1	2.05	0.74
2:B:518:ASP:CG	3:I:327:LYS:HZ2	1.95	0.74
2:B:603:ILE:CG1	3:I:239:THR:HG21	2.18	0.72
1:A:336:ALA:HB3	1:A:354:PHE:HB3	1.70	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:PRO:O	1:A:458:VAL:CG2	2.37	0.72
2:B:603:ILE:HG13	3:I:239:THR:HG21	1.68	0.72
1:A:358:CYS:SG	1:A:359:GLN:N	2.63	0.72
2:B:518:ASP:CB	3:I:327:LYS:CE	2.68	0.72
1:A:449:PRO:CB	2:B:569:LEU:HD11	2.21	0.71
3:I:277:LEU:HB2	3:I:309:ILE:CG2	2.21	0.71
3:I:343:VAL:O	3:I:347:ILE:HG13	1.91	0.71
3:I:227:ILE:HG21	3:I:337:ARG:HB2	1.73	0.70
2:B:522:GLY:HA2	2:B:573:LEU:HD13	1.74	0.69
2:B:642:HIS:CD2	2:B:643:PRO:HD2	2.27	0.69
2:B:479:VAL:HG12	2:B:480:PHE:H	1.57	0.69
1:A:452:GLY:N	2:B:575:PRO:O	2.26	0.69
2:B:649:ALA:C	3:I:248:ARG:HH21	1.99	0.69
1:A:323:ASN:OD1	1:A:323:ASN:O	2.11	0.68
2:B:602:LYS:HG2	2:B:603:ILE:H	1.57	0.68
1:A:323:ASN:ND2	1:A:335:ILE:HG12	2.09	0.68
1:A:457:PRO:CB	2:B:668:TRP:NE1	2.58	0.67
3:I:290:PHE:HB3	3:I:295:ASP:HB3	1.75	0.67
3:I:213:LEU:CD2	3:I:290:PHE:CZ	2.74	0.66
2:B:603:ILE:HG22	2:B:604:ALA:N	2.11	0.65
1:A:331:ARG:HH11	1:A:331:ARG:HB2	1.62	0.65
2:B:523:HIS:HB3	2:B:529:LEU:HG	1.79	0.64
3:I:250:ASP:O	3:I:254:LYS:HG3	1.97	0.64
2:B:642:HIS:ND1	2:B:644:SER:OG	2.30	0.64
2:B:602:LYS:HG2	2:B:603:ILE:N	2.12	0.63
1:A:449:PRO:HG2	2:B:493:GLY:HA2	1.80	0.63
1:A:346:GLU:O	1:A:346:GLU:HG2	1.99	0.62
2:B:594:SER:HB3	2:B:607:LEU:HD11	1.82	0.62
1:A:357:VAL:O	1:A:365:HIS:NE2	2.33	0.61
3:I:215:GLY:O	3:I:219:ASN:ND2	2.33	0.61
1:A:457:PRO:HB2	2:B:668:TRP:CZ2	2.36	0.60
1:A:451:CYS:HA	2:B:575:PRO:HG2	1.81	0.60
1:A:454:PRO:HG2	1:A:457:PRO:CD	2.31	0.60
3:I:290:PHE:CB	3:I:295:ASP:HB3	2.30	0.60
3:I:273:PHE:HD2	3:I:313:ILE:HG12	1.67	0.60
3:I:234:TYR:HB2	3:I:326:TYR:CD2	2.37	0.60
2:B:518:ASP:CB	3:I:327:LYS:NZ	2.66	0.59
1:A:411:TYR:CZ	2:B:569:LEU:HG	2.37	0.59
2:B:603:ILE:CG2	2:B:604:ALA:H	2.16	0.58
1:A:457:PRO:HB3	2:B:668:TRP:NE1	2.19	0.58
2:B:601:GLU:O	2:B:601:GLU:HG2	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:651:GLN:HG3	3:I:242:THR:HG22	1.85	0.58
1:A:310:PRO:O	1:A:364:TRP:NE1	2.36	0.58
1:A:457:PRO:C	1:A:458:VAL:HG23	2.28	0.58
2:B:518:ASP:HB3	3:I:327:LYS:NZ	2.19	0.58
2:B:579:PRO:HG3	2:B:671:THR:HA	1.86	0.58
3:I:234:TYR:HB2	3:I:326:TYR:HD2	1.69	0.57
2:B:581:ASN:HB3	2:B:583:THR:HG23	1.87	0.57
1:A:314:THR:HG22	1:A:321:ILE:HD11	1.86	0.57
2:B:603:ILE:HG22	2:B:604:ALA:H	1.70	0.56
2:B:495:ARG:HD3	2:B:703:GLU:OE2	2.05	0.56
2:B:530:MET:O	3:I:331:THR:HG23	2.06	0.56
2:B:603:ILE:CG2	2:B:604:ALA:N	2.68	0.56
2:B:479:VAL:HG22	2:B:521:LEU:HD21	1.87	0.56
1:A:346:GLU:CB	1:A:369:PRO:HB3	2.32	0.56
1:A:457:PRO:CB	2:B:668:TRP:HE1	2.17	0.56
1:A:449:PRO:HB3	2:B:569:LEU:HD11	1.87	0.56
3:I:347:ILE:O	3:I:347:ILE:HG22	2.04	0.56
1:A:346:GLU:CD	1:A:366:ARG:HG2	2.31	0.56
2:B:539:ARG:HB3	2:B:562:GLU:HB3	1.87	0.56
2:B:613:PRO:HD2	2:B:645:LEU:HD11	1.87	0.55
1:A:422:SER:O	1:A:422:SER:OG	2.18	0.55
1:A:449:PRO:HG3	2:B:493:GLY:C	2.32	0.55
2:B:635:GLN:C	2:B:637:MET:H	2.13	0.55
1:A:360:ASP:OD1	1:A:360:ASP:N	2.38	0.55
2:B:472:MET:HE3	2:B:524:THR:HG23	1.87	0.55
1:A:387:PHE:HE2	1:A:389:TYR:HE1	1.54	0.55
1:A:454:PRO:HG2	1:A:457:PRO:CA	2.37	0.55
2:B:480:PHE:HB3	2:B:520:PHE:HB2	1.88	0.55
3:I:274:LYS:O	3:I:278:ASN:HB2	2.07	0.54
2:B:500:ALA:HA	2:B:673:ILE:HD11	1.90	0.54
2:B:518:ASP:HB2	3:I:327:LYS:HE3	1.86	0.53
2:B:673:ILE:CG2	2:B:688:THR:CB	2.76	0.53
1:A:437:ASN:OD1	1:A:438:GLU:N	2.41	0.53
2:B:602:LYS:CG	2:B:603:ILE:H	2.20	0.53
1:A:457:PRO:HB2	2:B:668:TRP:CE2	2.44	0.52
2:B:518:ASP:HB3	3:I:327:LYS:HZ1	1.74	0.52
2:B:583:THR:C	2:B:585:TYR:N	2.67	0.52
2:B:478:GLN:NE2	2:B:479:VAL:O	2.42	0.52
2:B:585:TYR:HE2	2:B:689:LYS:HB2	1.75	0.52
3:I:290:PHE:HB3	3:I:295:ASP:CB	2.40	0.52
2:B:530:MET:HE1	3:I:234:TYR:CE1	2.45	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:583:THR:C	2:B:585:TYR:H	2.17	0.52
1:A:330:PHE:C	1:A:332:ASP:H	2.18	0.51
2:B:495:ARG:HD3	2:B:703:GLU:CD	2.34	0.51
3:I:230:ILE:HD13	3:I:273:PHE:HE1	1.75	0.51
3:I:276:LEU:CD2	3:I:309:ILE:HD11	2.40	0.51
2:B:477:TRP:HB2	2:B:491:LEU:H	1.76	0.51
2:B:647:GLN:N	2:B:647:GLN:OE1	2.44	0.51
2:B:635:GLN:C	2:B:637:MET:N	2.68	0.51
3:I:213:LEU:O	3:I:217:LYS:N	2.41	0.51
1:A:354:PHE:CE2	1:A:356:ALA:HB2	2.46	0.50
1:A:457:PRO:HB2	2:B:668:TRP:NE1	2.25	0.50
1:A:412:LYS:HB2	1:A:450:VAL:HG22	1.92	0.50
2:B:538:ARG:HB3	2:B:562:GLU:HG2	1.94	0.50
1:A:456:ASN:O	2:B:474:ASN:HA	2.12	0.50
2:B:577:CYS:HB2	2:B:668:TRP:O	2.11	0.50
3:I:213:LEU:C	3:I:215:GLY:H	2.20	0.49
2:B:641:GLY:HA2	2:B:645:LEU:HD12	1.94	0.49
1:A:454:PRO:HD2	2:B:668:TRP:CD1	2.47	0.49
3:I:327:LYS:C	3:I:329:ILE:H	2.19	0.49
3:I:251:ASN:HA	3:I:254:LYS:HB2	1.94	0.49
3:I:327:LYS:C	3:I:329:ILE:N	2.70	0.49
1:A:323:ASN:HD21	1:A:335:ILE:HG12	1.77	0.49
3:I:240:LYS:HD2	3:I:260:GLU:OE1	2.13	0.48
2:B:538:ARG:HB2	2:B:564:GLU:HA	1.95	0.48
3:I:224:ILE:HG23	3:I:337:ARG:HG3	1.94	0.48
3:I:273:PHE:C	3:I:275:THR:N	2.69	0.48
2:B:602:LYS:CG	2:B:603:ILE:N	2.77	0.48
1:A:455:VAL:HG21	2:B:571:PRO:HB2	1.94	0.48
2:B:694:VAL:HG12	2:B:698:LYS:HE2	1.95	0.48
3:I:333:ILE:HA	3:I:336:MET:HB3	1.96	0.48
2:B:479:VAL:HG13	2:B:521:LEU:HG	1.94	0.47
3:I:343:VAL:O	3:I:347:ILE:CG1	2.60	0.47
3:I:313:ILE:O	3:I:317:LYS:HG2	2.15	0.47
1:A:334:PHE:CE1	1:A:356:ALA:HB3	2.50	0.47
1:A:427:TYR:OH	1:A:443:LYS:O	2.24	0.47
2:B:581:ASN:O	2:B:691:LEU:CD1	2.63	0.47
2:B:643:PRO:HD3	2:B:684:TYR:CE2	2.50	0.46
1:A:330:PHE:O	1:A:332:ASP:N	2.49	0.46
2:B:585:TYR:CE2	2:B:689:LYS:HB2	2.49	0.46
2:B:651:GLN:HG2	3:I:246:SER:OG	2.15	0.46
2:B:635:GLN:HG2	2:B:635:GLN:O	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:312:LEU:HD22	3:I:329:ILE:HG22	1.97	0.46
2:B:476:PRO:HB2	2:B:574:LEU:H	1.80	0.46
3:I:220:VAL:HG13	3:I:340:LEU:HD22	1.98	0.46
1:A:437:ASN:ND2	1:A:440:LYS:HD3	2.30	0.46
1:A:449:PRO:HB2	2:B:569:LEU:HD11	1.97	0.46
1:A:309:CYS:N	1:A:328:TYR:O	2.48	0.46
2:B:464:ILE:O	2:B:599:MET:HA	2.15	0.46
2:B:603:ILE:HG12	3:I:239:THR:CB	2.46	0.46
2:B:502:HIS:CE1	2:B:654:SER:HB2	2.50	0.46
1:A:344:LEU:HD12	1:A:351:LEU:HB2	1.97	0.46
1:A:438:GLU:OE1	1:A:439:GLN:NE2	2.49	0.46
3:I:338:ASP:HA	3:I:341:LYS:HG3	1.97	0.46
3:I:217:LYS:HD2	3:I:347:ILE:CG2	2.46	0.45
1:A:398:TYR:CG	1:A:399:LYS:HG3	2.52	0.45
2:B:496:TRP:CZ3	2:B:562:GLU:HB2	2.51	0.45
3:I:273:PHE:C	3:I:275:THR:H	2.24	0.45
1:A:427:TYR:CZ	1:A:437:ASN:HB2	2.51	0.45
1:A:449:PRO:CG	2:B:493:GLY:C	2.89	0.45
2:B:530:MET:SD	3:I:330:VAL:HG22	2.56	0.45
1:A:322:GLN:O	1:A:323:ASN:CG	2.60	0.45
1:A:346:GLU:OE2	1:A:366:ARG:HG3	2.12	0.45
2:B:649:ALA:CB	3:I:248:ARG:NH2	2.77	0.45
3:I:216:VAL:HG13	3:I:217:LYS:N	2.31	0.45
2:B:629:ARG:NE	2:B:678:ILE:HD11	2.32	0.45
3:I:217:LYS:HD2	3:I:347:ILE:HG21	1.98	0.45
3:I:256:LYS:HD3	3:I:256:LYS:HA	1.76	0.45
1:A:454:PRO:HG3	1:A:457:PRO:HB3	1.95	0.44
2:B:543:HIS:ND1	2:B:545:ASP:HB2	2.31	0.44
2:B:634:SER:O	2:B:637:MET:HB2	2.17	0.44
2:B:691:LEU:HA	2:B:694:VAL:HG23	2.00	0.44
1:A:449:PRO:HB2	2:B:493:GLY:O	2.17	0.44
1:A:343:GLN:HB2	1:A:374:LYS:HG2	1.98	0.44
1:A:454:PRO:HG2	1:A:457:PRO:HD3	1.98	0.44
2:B:523:HIS:ND1	2:B:528:GLU:HB2	2.32	0.44
1:A:355:THR:O	1:A:355:THR:OG1	2.30	0.44
3:I:212:TYR:O	3:I:216:VAL:HG12	2.18	0.44
2:B:603:ILE:CG1	3:I:239:THR:CG2	2.92	0.43
3:I:329:ILE:O	3:I:333:ILE:HG12	2.19	0.43
2:B:494:ASP:OD2	2:B:566:SER:HB2	2.18	0.43
1:A:451:CYS:HB2	2:B:576:ILE:C	2.43	0.43
1:A:454:PRO:HG2	1:A:457:PRO:CG	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:479:VAL:HG12	2:B:480:PHE:N	2.31	0.43
1:A:331:ARG:HH11	1:A:331:ARG:CG	2.28	0.43
2:B:622:ASN:OD1	2:B:625:ARG:NH2	2.52	0.43
1:A:435:TRP:O	1:A:442:GLU:HA	2.19	0.43
3:I:226:THR:O	3:I:230:ILE:HG13	2.18	0.42
1:A:408:GLU:HA	1:A:409:PRO:HA	1.71	0.42
1:A:457:PRO:CB	2:B:668:TRP:CE2	3.02	0.42
2:B:633:PHE:O	2:B:633:PHE:CG	2.73	0.42
3:I:277:LEU:CB	3:I:309:ILE:HG21	2.38	0.42
3:I:305:ILE:HG23	3:I:336:MET:HE2	2.01	0.42
1:A:424:GLN:HG2	1:A:439:GLN:CD	2.44	0.42
2:B:481:THR:HB	2:B:483:ILE:HG13	2.02	0.42
2:B:585:TYR:N	2:B:585:TYR:CD1	2.88	0.42
1:A:454:PRO:HB2	2:B:473:GLY:O	2.19	0.42
1:A:379:PRO:HB3	1:A:404:TYR:OH	2.19	0.42
3:I:280:ILE:HD11	3:I:340:LEU:HD11	2.01	0.42
2:B:477:TRP:CE2	2:B:576:ILE:HD12	2.55	0.41
3:I:290:PHE:CD2	3:I:295:ASP:CB	2.91	0.41
2:B:673:ILE:HG22	2:B:688:THR:HB	1.88	0.41
1:A:323:ASN:HD21	1:A:334:PHE:HA	1.83	0.41
1:A:348:ASN:O	1:A:348:ASN:ND2	2.53	0.41
3:I:312:LEU:HD11	3:I:332:SER:OG	2.20	0.41
3:I:243:GLN:C	3:I:246:SER:HG	2.28	0.41
1:A:387:PHE:HB3	1:A:404:TYR:HA	2.03	0.41
2:B:676:TRP:HB2	3:I:247:THR:HB	2.03	0.41
3:I:240:LYS:HA	3:I:240:LYS:HD3	1.81	0.41
2:B:670:ALA:O	2:B:690:VAL:HG11	2.20	0.40
2:B:573:LEU:HD12	2:B:573:LEU:HA	1.77	0.40
1:A:331:ARG:CG	1:A:331:ARG:NH1	2.84	0.40
2:B:536:PRO:HB2	2:B:564:GLU:HB2	2.03	0.40
3:I:213:LEU:C	3:I:215:GLY:N	2.77	0.40
2:B:603:ILE:HG12	3:I:239:THR:CG2	2.52	0.40
1:A:454:PRO:C	1:A:456:ASN:N	2.79	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	136/164 (83%)	108 (79%)	28 (21%)	0	100	100
2	B	227/242 (94%)	189 (83%)	37 (16%)	1 (0%)	30	65
3	I	136/148 (92%)	121 (89%)	15 (11%)	0	100	100
All	All	499/554 (90%)	418 (84%)	80 (16%)	1 (0%)	43	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	655	GLY

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	127/147 (86%)	126 (99%)	1 (1%)	73	78
2	B	194/202 (96%)	193 (100%)	1 (0%)	81	82
3	I	123/131 (94%)	121 (98%)	2 (2%)	55	70
All	All	444/480 (92%)	440 (99%)	4 (1%)	70	77

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	331	ARG
2	B	586	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	I	248	ARG
3	I	326	TYR

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

Mol	Chain	Res	Type
1	A	311	GLN
1	A	348	ASN
2	B	565	ASN
3	I	232	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](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	B	801	2	14,14,15	0.29	0	17,19,21	0.57	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	801	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	801	NAG	C8-C7-N2-C2
4	B	801	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

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	142/164 (86%)	0.78	13 (9%) 14 17	94, 113, 140, 161	0
2	B	233/242 (96%)	1.05	30 (12%) 7 11	68, 100, 129, 141	0
3	I	138/148 (93%)	1.07	22 (15%) 5 8	72, 106, 152, 160	0
All	All	513/554 (92%)	0.98	65 (12%) 8 11	68, 106, 140, 161	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	284	VAL	5.2
2	B	692	ASN	5.0
2	B	559	ALA	4.8
2	B	648	ASP	4.7
3	I	343	VAL	4.7
2	B	631	ASP	4.6
3	I	245	TYR	4.3
3	I	211	SER	4.1
2	B	638	PHE	3.9
2	B	508	GLU	3.9
1	A	312	PRO	3.9
3	I	238	SER	3.9
2	B	636	ASN	3.9
2	B	558	ILE	3.8
1	A	372	LYS	3.5
3	I	342	GLU	3.4
2	B	554	PHE	3.3
2	B	703	GLU	3.3
1	A	402	ILE	3.3
1	A	425	GLY	3.2
2	B	684	TYR	3.2
3	I	291	VAL	3.2
1	A	450	VAL	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	605	HIS	2.9
1	A	458	VAL	2.9
2	B	635	GLN	2.9
3	I	344	GLN	2.9
2	B	649	ALA	2.8
2	B	678	ILE	2.8
3	I	309	ILE	2.7
3	I	214	GLU	2.7
2	B	654	SER	2.7
2	B	578	LEU	2.7
1	A	335	ILE	2.6
1	A	457	PRO	2.6
2	B	505	TYR	2.6
3	I	289	ASN	2.6
3	I	268	ASP	2.6
3	I	225	GLN	2.5
2	B	653	ASP	2.5
2	B	482	ASN	2.5
3	I	320	SER	2.4
2	B	627	LYS	2.4
2	B	597	GLY	2.4
3	I	277	LEU	2.4
2	B	604	ALA	2.4
2	B	662	ASP	2.4
1	A	316	ASP	2.3
2	B	556	GLY	2.3
3	I	297	HIS	2.3
3	I	241	LEU	2.3
2	B	580	ASP	2.2
3	I	273	PHE	2.2
2	B	507	LYS	2.1
1	A	424	GLN	2.1
1	A	313	LYS	2.1
3	I	252	PHE	2.1
1	A	323	ASN	2.1
2	B	670	ALA	2.1
3	I	231	TYR	2.1
1	A	365	HIS	2.0
2	B	677	GLY	2.0
2	B	557	ASP	2.0
3	I	217	LYS	2.0
3	I	306	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	B	801	14/15	0.60	0.12	120,133,138,139	0

6.5 Other polymers [i](#)

There are no such residues in this entry.