



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:07 AM UTC

PDB ID : 1QS1 / pdb_00001qs1
Title : CRYSTAL STRUCTURE OF VEGETATIVE INSECTICIDAL PROTEIN2 (VIP2)
Authors : Han, S.; Craig, J.A.; Putnam, C.D.; Carozzi, N.B.; Tainer, J.A.
Deposited on : 1999-06-25
Resolution : 1.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

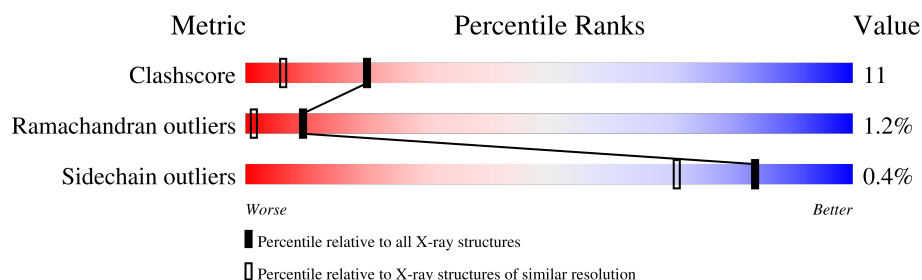
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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))
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	462	70% 16% • 13%
1	B	462	65% 21% • 13%
1	C	462	65% 21% • 13%
1	D	462	70% 15% • 13%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14325 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 ADP-RIBOSYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	402	Total	C	N	O	S	0	0	0
			3206	2024	533	638	11			
1	B	402	Total	C	N	O	S	0	0	0
			3206	2024	533	638	11			
1	C	402	Total	C	N	O	S	0	0	0
			3206	2024	533	638	11			
1	D	402	Total	C	N	O	S	0	0	0
			3206	2024	533	638	11			

- Molecule 2 is water.

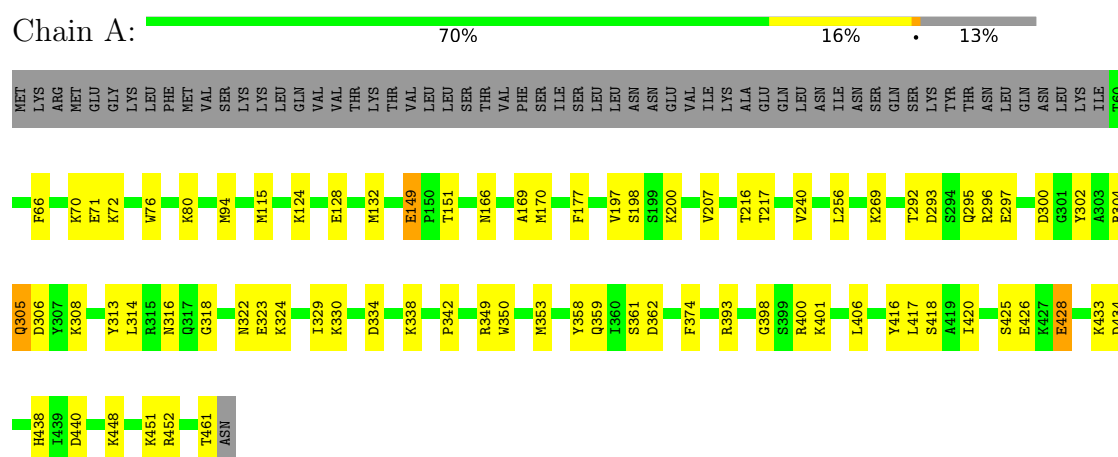
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	406	Total	O	0	0
			406	406		
2	B	377	Total	O	0	0
			377	377		
2	C	344	Total	O	0	0
			344	344		
2	D	374	Total	O	0	0
			374	374		

3 Residue-property plots

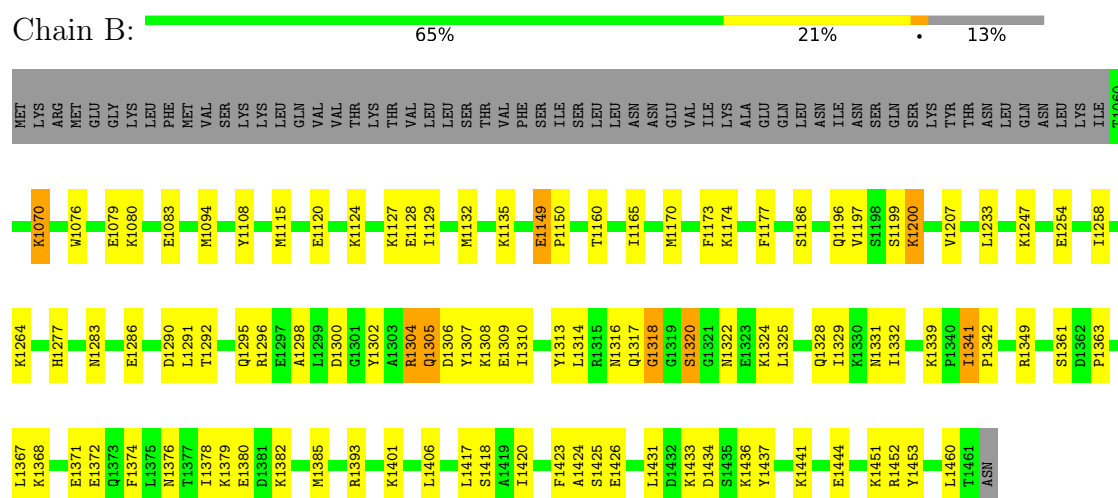
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

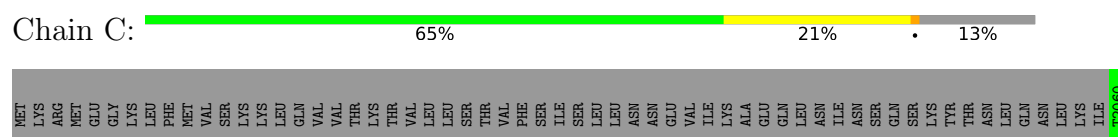
• Molecule 1: ADP-RIBOSYLTRANSFERASE

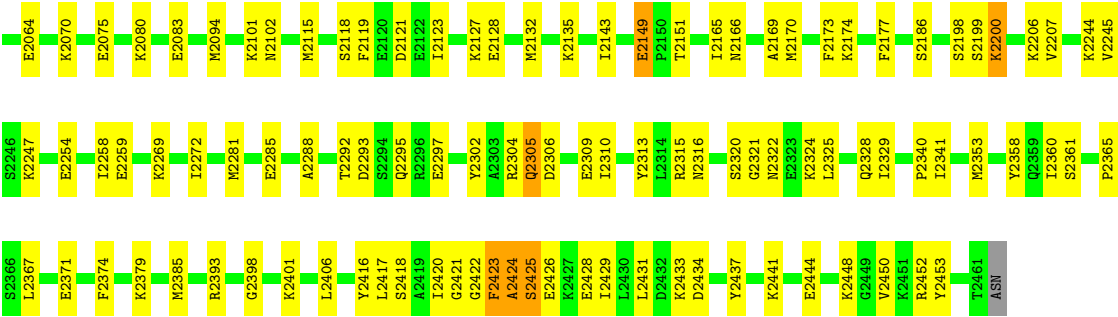


• Molecule 1: ADP-RIBOSYLTRANSFERASE

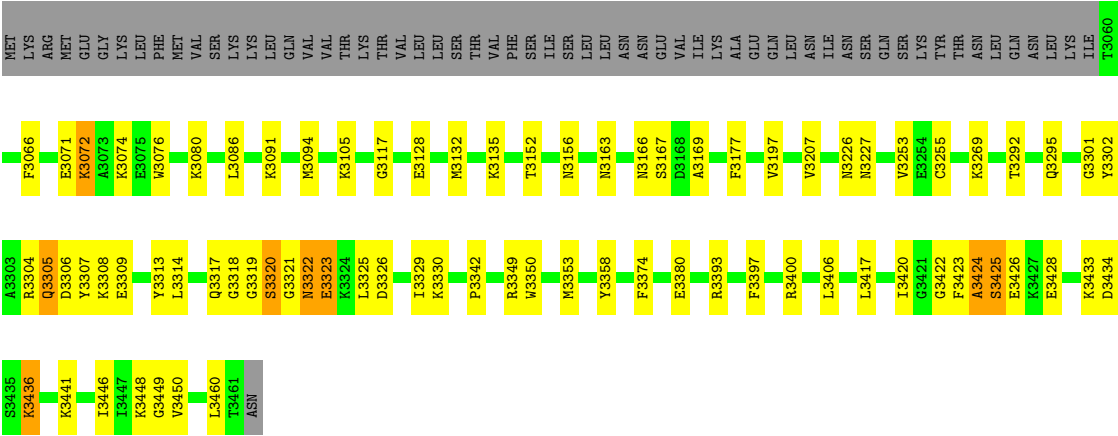


• Molecule 1: ADP-RIBOSYLTRANSFERASE





● Molecule 1: ADP-RIBOSYLTRANSFERASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	53.90Å 78.70Å 105.90Å 108.65° 89.96° 90.02°	Depositor
Resolution (Å)	20.00 – 1.50	Depositor
% Data completeness (in resolution range)	81.4 (20.00-1.50)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.235 , 0.269	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14325	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

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	0.36	0/3258	0.87	8/4376 (0.2%)
1	B	0.35	0/3258	0.86	8/4376 (0.2%)
1	C	0.34	0/3258	0.88	11/4376 (0.3%)
1	D	0.36	0/3258	0.86	8/4376 (0.2%)
All	All	0.35	0/13032	0.87	35/17504 (0.2%)

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2341	ILE	CA-C-N	7.16	127.15	119.28
1	C	2341	ILE	C-N-CA	7.16	127.15	119.28
1	A	374	PHE	N-CA-C	7.01	122.74	114.04
1	D	3207	VAL	N-CA-C	6.88	117.78	107.80
1	C	2177	PHE	N-CA-C	6.81	122.26	113.88
1	C	2269	LYS	CB-CA-C	-6.79	108.73	116.54
1	A	207	VAL	N-CA-C	6.64	117.69	107.99
1	B	1207	VAL	N-CA-C	6.61	117.64	107.99
1	D	3374	PHE	N-CA-C	6.60	122.23	114.04
1	C	2207	VAL	N-CA-C	6.58	117.60	107.99
1	A	428	GLU	N-CA-C	6.53	120.30	109.46
1	B	1341	ILE	CA-C-N	6.44	126.13	119.56
1	B	1341	ILE	C-N-CA	6.44	126.13	119.56
1	B	1149	GLU	N-CA-C	-6.35	102.05	109.93
1	D	3406	LEU	N-CA-C	6.35	119.58	109.24
1	C	2424	ALA	N-CA-C	-6.33	105.14	112.86
1	B	1406	LEU	N-CA-C	6.29	119.50	109.24
1	D	3269	LYS	CB-CA-C	-6.23	109.38	116.54
1	C	2374	PHE	N-CA-C	6.05	121.54	114.04
1	B	1083	GLU	N-CA-C	6.05	118.83	111.82
1	B	1374	PHE	N-CA-C	6.01	122.07	114.31
1	A	269	LYS	CB-CA-C	-5.99	109.65	116.54
1	B	1177	PHE	N-CA-C	5.95	121.98	114.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	3342	PRO	N-CA-C	5.87	121.48	113.84
1	D	3177	PHE	N-CA-C	5.72	121.29	113.97
1	A	177	PHE	N-CA-C	5.71	121.27	113.97
1	D	3428	GLU	N-CA-C	5.69	118.91	109.46
1	C	2406	LEU	N-CA-C	5.56	118.30	109.24
1	C	2428	GLU	N-CA-C	5.55	118.97	110.20
1	A	406	LEU	N-CA-C	5.54	118.27	109.24
1	C	2398	GLY	N-CA-C	5.35	119.36	112.83
1	C	2149	GLU	N-CA-C	-5.33	103.33	109.93
1	A	342	PRO	N-CA-C	5.26	120.68	113.84
1	D	3156	ASN	N-CA-C	5.25	118.71	112.72
1	A	149	GLU	N-CA-C	-5.09	103.62	109.93

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3206	0	3209	55	0
1	B	3206	0	3209	83	0
1	C	3206	0	3209	90	0
1	D	3206	0	3209	69	0
2	A	406	0	0	12	0
2	B	377	0	0	12	0
2	C	344	0	0	11	0
2	D	374	0	0	11	0
All	All	14325	0	12836	293	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 11.

All (293) 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:C:2094:MET:HE3	1:C:2094:MET:HA	1.46	0.97
1:B:1378:ILE:HD12	1:B:1460:LEU:HD11	1.53	0.89
1:D:3066:PHE:HE2	1:D:3072:LYS:HD2	1.41	0.85
1:A:296:ARG:NH1	1:A:420:ILE:HB	1.94	0.83
1:D:3066:PHE:CE2	1:D:3072:LYS:HD2	2.14	0.82
1:C:2385:MET:HE3	1:C:2431:LEU:HD12	1.60	0.82
1:B:1170:MET:SD	1:B:1247:LYS:HE3	2.21	0.81
1:B:1296:ARG:HH11	1:B:1296:ARG:HB2	1.48	0.79
1:C:2173:PHE:CZ	1:C:2258:ILE:HD11	2.19	0.77
1:B:1296:ARG:HB2	1:B:1296:ARG:NH1	2.01	0.76
1:D:3105:LYS:HG3	2:D:6799:HOH:O	1.86	0.76
1:A:292:THR:OG1	1:A:295:GLN:HG3	1.84	0.76
1:B:1160:THR:HG22	1:B:1165:ILE:HD13	1.67	0.76
1:C:2281:MET:O	1:C:2285:GLU:HG3	1.87	0.74
1:D:3446:ILE:HD12	1:D:3450:VAL:C	2.13	0.74
1:B:1304:ARG:HB3	1:B:1305:GLN:NE2	2.03	0.73
1:C:2360:ILE:HD12	1:C:2361:SER:N	2.02	0.73
1:B:1292:THR:OG1	1:B:1295:GLN:HG2	1.89	0.73
1:D:3292:THR:OG1	1:D:3295:GLN:HG3	1.88	0.72
1:B:1300:ASP:O	1:B:1304:ARG:HG3	1.90	0.72
1:B:1368:LYS:O	1:B:1372:GLU:HG3	1.90	0.71
1:C:2173:PHE:HZ	1:C:2258:ILE:HD11	1.54	0.71
1:C:2393:ARG:HH22	1:C:2448:LYS:HD3	1.55	0.71
1:A:293:ASP:O	1:A:297:GLU:HG3	1.91	0.71
1:A:401:LYS:HE2	1:C:2121:ASP:OD2	1.92	0.69
1:C:2292:THR:OG1	1:C:2295:GLN:HG3	1.93	0.69
1:D:3446:ILE:HG22	2:D:4961:HOH:O	1.93	0.68
1:D:3094:MET:HE3	1:D:3094:MET:HA	1.76	0.68
1:D:3322:ASN:HB3	2:D:6997:HOH:O	1.95	0.67
1:A:302:TYR:HA	1:A:306:ASP:HB2	1.77	0.67
1:B:1124:LYS:HD3	2:B:4399:HOH:O	1.95	0.67
1:B:1173:PHE:CZ	1:B:1258:ILE:HD11	2.31	0.66
1:D:3326:ASP:O	1:D:3330:LYS:HG3	1.95	0.66
1:D:3163:ASN:ND2	1:D:3253:VAL:HG22	2.12	0.65
1:B:1197:VAL:HG12	2:B:6916:HOH:O	1.95	0.65
1:C:2281:MET:HE3	1:C:2285:GLU:HG2	1.77	0.65
1:D:3423:PHE:O	1:D:3425:SER:N	2.30	0.65
1:D:3441:LYS:HE3	2:D:4197:HOH:O	1.96	0.64
1:C:2441:LYS:HE3	2:C:4177:HOH:O	1.98	0.64
1:A:316:ASN:HB3	2:A:6906:HOH:O	1.97	0.64
1:D:3397:PHE:O	1:D:3400:ARG:HD3	1.97	0.64
1:B:1322:ASN:OD1	1:B:1325:LEU:HG	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1304:ARG:HB3	1:B:1305:GLN:HE22	1.63	0.64
1:B:1094:MET:HE1	1:B:1129:ILE:HG23	1.80	0.63
1:C:2293:ASP:O	1:C:2297:GLU:HB2	1.97	0.63
1:C:2247:LYS:HD3	1:C:2254:GLU:CD	2.24	0.62
1:B:1441:LYS:HE3	2:B:4100:HOH:O	1.98	0.62
1:C:2324:LYS:HB3	2:C:6987:HOH:O	1.99	0.62
1:A:200:LYS:NZ	1:A:200:LYS:HB3	2.15	0.62
1:C:2421:GLY:C	1:C:2423:PHE:H	2.07	0.62
1:A:170:MET:HG2	1:A:256:LEU:HD21	1.81	0.62
1:B:1426:GLU:N	1:B:1426:GLU:OE1	2.33	0.62
1:B:1296:ARG:HH11	1:B:1296:ARG:CB	2.14	0.61
1:B:1313:TYR:HE1	1:B:1320:SER:HB3	1.65	0.61
1:D:3325:LEU:HB2	2:D:6997:HOH:O	1.99	0.61
1:C:2080:LYS:O	1:C:2083:GLU:HG2	2.01	0.61
1:D:3349:ARG:HG2	1:D:3349:ARG:HH11	1.66	0.60
1:A:94:MET:HE2	1:A:132:MET:SD	2.41	0.60
1:D:3314:LEU:HD21	1:D:3329:ILE:HD13	1.81	0.60
1:D:3301:GLY:HA2	1:D:3304:ARG:HH12	1.66	0.60
1:B:1304:ARG:HG2	1:B:1423:PHE:CD2	2.36	0.59
1:A:362:ASP:HB2	2:A:6863:HOH:O	2.01	0.59
1:D:3132:MET:O	1:D:3135:LYS:HG2	2.02	0.59
1:B:1380:GLU:OE1	1:B:1436:LYS:HE3	2.02	0.59
1:A:197:VAL:HA	2:A:5114:HOH:O	2.02	0.58
1:B:1127:LYS:NZ	1:B:1127:LYS:HB3	2.18	0.58
1:A:353:MET:HE2	2:A:6863:HOH:O	2.01	0.58
1:A:426:GLU:CD	1:A:426:GLU:H	2.11	0.58
1:C:2444:GLU:HG2	1:C:2453:TYR:CE2	2.38	0.58
1:A:349:ARG:HG2	1:A:349:ARG:HH11	1.68	0.58
1:D:3350:TRP:CH2	1:D:3393:ARG:HD3	2.38	0.58
1:C:2325:LEU:O	1:C:2329:ILE:HG12	2.04	0.58
1:B:1349:ARG:HG2	1:B:1349:ARG:HH11	1.67	0.57
1:B:1173:PHE:HZ	1:B:1258:ILE:HD11	1.69	0.57
1:C:2199:SER:O	1:C:2200:LYS:HB2	2.05	0.57
1:D:3436:LYS:NZ	1:D:3460:LEU:HD12	2.20	0.57
1:B:1132:MET:O	1:B:1135:LYS:HG2	2.05	0.57
1:D:3446:ILE:HD11	1:D:3449:GLY:C	2.30	0.57
1:C:2094:MET:HA	1:C:2094:MET:CE	2.28	0.56
1:C:2417:LEU:HD13	1:C:2417:LEU:O	2.06	0.56
1:D:3436:LYS:HZ3	1:D:3460:LEU:HD12	1.70	0.56
1:B:1309:GLU:HB3	2:B:6775:HOH:O	2.05	0.56
1:D:3309:GLU:OE2	1:D:3325:LEU:HD21	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:ASN:HB3	1:A:169:ALA:HB2	1.86	0.56
1:C:2401:LYS:HA	1:C:2452:ARG:CD	2.36	0.55
1:A:296:ARG:HH12	1:A:420:ILE:HB	1.68	0.55
1:D:3422:GLY:O	1:D:3423:PHE:HB3	2.06	0.55
1:D:3446:ILE:HG23	1:D:3446:ILE:O	2.05	0.55
1:C:2315:ARG:C	1:C:2316:ASN:HD22	2.14	0.55
1:B:1170:MET:O	1:B:1174:LYS:HG3	2.08	0.54
1:C:2288:ALA:HB1	1:C:2420:ILE:HA	1.88	0.54
1:B:1298:ALA:HA	1:B:1328:GLN:HE21	1.73	0.54
1:B:1316:ASN:O	1:B:1317:GLN:HB2	2.07	0.54
1:B:1417:LEU:HD13	1:B:1417:LEU:O	2.08	0.54
1:C:2310:ILE:HD11	1:C:2328:GLN:NE2	2.23	0.54
1:A:240:VAL:HG23	2:A:4683:HOH:O	2.07	0.54
1:B:1307:TYR:CE1	1:B:1308:LYS:HG3	2.43	0.54
1:D:3086:LEU:O	1:D:3091:LYS:NZ	2.40	0.54
1:B:1070:LYS:HB2	1:B:1070:LYS:NZ	2.23	0.53
1:D:3426:GLU:CD	1:D:3426:GLU:H	2.17	0.53
1:D:3326:ASP:HB3	1:D:3330:LYS:NZ	2.23	0.53
1:D:3080:LYS:HD2	1:D:3080:LYS:N	2.24	0.53
1:A:400:ARG:HG2	2:A:6503:HOH:O	2.07	0.53
1:B:1322:ASN:C	1:B:1322:ASN:HD22	2.16	0.53
1:A:361:SER:O	1:C:2118:SER:HA	2.09	0.53
1:D:3423:PHE:O	1:D:3424:ALA:C	2.52	0.53
1:D:3166:ASN:HB2	1:D:3169:ALA:HB3	1.91	0.52
1:B:1170:MET:SD	1:B:1247:LYS:HG3	2.49	0.52
1:D:3400:ARG:HG3	1:D:3400:ARG:HH11	1.73	0.52
1:C:2247:LYS:HD3	1:C:2254:GLU:OE2	2.10	0.52
1:C:2304:ARG:HG3	1:C:2305:GLN:HG2	1.91	0.52
1:A:66:PHE:CE2	1:A:72:LYS:HG2	2.43	0.52
1:B:1094:MET:SD	1:B:1233:LEU:HD21	2.50	0.52
1:B:1418:SER:HA	1:B:1424:ALA:HB1	1.92	0.52
1:C:2393:ARG:HH22	1:C:2448:LYS:CD	2.22	0.52
1:A:149:GLU:OE1	1:A:151:THR:OG1	2.23	0.52
1:C:2313:TYR:CE1	1:C:2320:SER:HB3	2.44	0.52
1:A:66:PHE:HE2	1:A:72:LYS:HG2	1.75	0.52
1:C:2450:VAL:HG12	1:C:2452:ARG:NH1	2.24	0.52
1:A:216:THR:HG23	1:A:217:THR:HG23	1.92	0.52
1:C:2420:ILE:HG13	1:C:2421:GLY:N	2.23	0.52
1:D:3313:TYR:HD1	1:D:3317:GLN:OE1	1.93	0.52
1:D:3417:LEU:O	1:D:3420:ILE:HG12	2.10	0.52
1:C:2244:LYS:NZ	1:C:2259:GLU:OE2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:HIS:HD2	1:A:440:ASP:OD1	1.94	0.51
1:B:1302:TYR:HD1	1:B:1310:ILE:HD12	1.75	0.51
1:B:1322:ASN:HD21	1:B:1324:LYS:HB2	1.76	0.51
1:C:2340:PRO:HG3	2:C:5328:HOH:O	2.10	0.51
1:A:323:GLU:HB2	2:A:6779:HOH:O	2.10	0.51
1:B:1376:ASN:HB3	2:B:5247:HOH:O	2.11	0.51
1:C:2119:PHE:O	1:C:2123:ILE:HG12	2.10	0.51
1:B:1444:GLU:HG2	1:B:1453:TYR:CE2	2.46	0.51
1:C:2115:MET:HE3	1:C:2393:ARG:NE	2.26	0.51
1:C:2401:LYS:HA	1:C:2452:ARG:HD3	1.93	0.51
1:C:2132:MET:O	1:C:2135:LYS:HG2	2.11	0.50
1:C:2143:ILE:HG21	1:C:2206:LYS:NZ	2.26	0.50
1:B:1385:MET:HE3	1:B:1431:LEU:HD12	1.91	0.50
1:A:425:SER:HB2	1:A:428:GLU:OE2	2.12	0.50
1:C:2309:GLU:OE1	1:C:2325:LEU:HD21	2.12	0.50
1:C:2165:ILE:HG12	1:C:2254:GLU:HG2	1.93	0.50
1:D:3436:LYS:NZ	1:D:3436:LYS:HB2	2.27	0.50
1:B:1128:GLU:O	1:B:1132:MET:HG3	2.12	0.50
1:B:1304:ARG:HG2	1:B:1423:PHE:CG	2.46	0.49
1:D:3301:GLY:HA2	1:D:3304:ARG:NH1	2.27	0.49
1:A:330:LYS:HG2	1:A:334:ASP:OD2	2.12	0.49
1:C:2173:PHE:CE2	1:C:2258:ILE:HD11	2.47	0.49
1:A:200:LYS:HB3	1:A:200:LYS:HZ3	1.77	0.49
1:B:1196:GLN:HA	1:B:1196:GLN:HE21	1.78	0.49
1:C:2174:LYS:HE2	2:C:6836:HOH:O	2.12	0.49
1:D:3321:GLY:O	1:D:3322:ASN:HB2	2.12	0.49
1:C:2115:MET:HE3	1:C:2393:ARG:NH2	2.28	0.49
1:C:2170:MET:SD	1:C:2247:LYS:HE3	2.53	0.49
1:C:2170:MET:O	1:C:2174:LYS:HG2	2.12	0.48
1:B:1328:GLN:O	1:B:1332:ILE:HG13	2.13	0.48
1:B:1094:MET:HE2	1:B:1132:MET:SD	2.53	0.48
1:D:3166:ASN:HB2	1:D:3169:ALA:CB	2.43	0.48
1:B:1283:ASN:O	1:B:1339:LYS:HE2	2.13	0.48
1:B:1305:GLN:HG3	2:C:6749:HOH:O	2.12	0.48
1:B:1076:TRP:O	1:B:1079:GLU:HG2	2.13	0.48
1:B:1417:LEU:O	1:B:1420:ILE:HG12	2.13	0.48
1:C:2423:PHE:C	1:C:2425:SER:N	2.70	0.48
1:B:1433:LYS:O	1:B:1434:ASP:HB2	2.13	0.48
1:C:2075:GLU:HB2	2:C:6945:HOH:O	2.12	0.48
1:B:1079:GLU:HG3	1:B:1080:LYS:N	2.29	0.48
1:C:2450:VAL:CG1	1:C:2452:ARG:NH1	2.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3074:LYS:HE3	2:D:4950:HOH:O	2.14	0.48
1:B:1385:MET:CE	1:B:1431:LEU:HD12	2.44	0.48
1:B:1314:LEU:HD21	1:B:1329:ILE:HD13	1.96	0.47
1:D:3308:LYS:HG2	2:D:4509:HOH:O	2.13	0.47
1:D:3086:LEU:HD23	1:D:3135:LYS:HD3	1.96	0.47
1:A:461:THR:HG23	2:A:5693:HOH:O	2.13	0.47
1:C:2325:LEU:HG	2:C:6987:HOH:O	2.14	0.47
1:C:2426:GLU:N	1:C:2426:GLU:OE2	2.47	0.47
1:B:1200:LYS:NZ	1:B:1200:LYS:HB3	2.28	0.47
1:A:76:TRP:O	1:A:80:LYS:HG2	2.15	0.47
1:B:1401:LYS:HG2	1:B:1452:ARG:HH12	1.79	0.47
1:D:3424:ALA:O	1:D:3425:SER:O	2.33	0.47
1:C:2379:LYS:HD3	1:C:2437:TYR:OH	2.15	0.47
1:C:2166:ASN:HB3	1:C:2169:ALA:HB2	1.96	0.47
1:A:417:LEU:O	1:A:420:ILE:HG12	2.15	0.46
1:B:1264:LYS:HG3	2:B:6834:HOH:O	2.14	0.46
1:C:2115:MET:HE3	1:C:2393:ARG:HE	1.80	0.46
1:D:3304:ARG:HG2	1:D:3305:GLN:OE1	2.15	0.46
1:B:1382:LYS:HD3	1:B:1434:ASP:OD2	2.15	0.46
1:C:2070:LYS:HG3	2:C:4453:HOH:O	2.14	0.46
1:C:2149:GLU:OE1	1:C:2151:THR:OG1	2.28	0.46
1:C:2313:TYR:HE1	1:C:2320:SER:HB3	1.79	0.46
1:A:433:LYS:O	1:A:434:ASP:HB2	2.15	0.46
1:C:2199:SER:O	1:C:2200:LYS:CB	2.63	0.46
1:C:2420:ILE:HG13	1:C:2422:GLY:H	1.81	0.46
1:B:1316:ASN:C	1:B:1318:GLY:H	2.24	0.45
1:D:3436:LYS:HE3	2:D:6020:HOH:O	2.16	0.45
1:D:3128:GLU:O	1:D:3132:MET:HG3	2.17	0.45
1:D:3304:ARG:HB2	1:D:3304:ARG:HH11	1.80	0.45
1:D:3380:GLU:HB3	1:D:3436:LYS:HG2	1.98	0.45
1:D:3167:SER:HB3	2:D:6937:HOH:O	2.16	0.45
1:D:3322:ASN:OD1	1:D:3323:GLU:N	2.36	0.45
1:A:426:GLU:CD	1:A:426:GLU:N	2.73	0.45
1:C:2421:GLY:C	1:C:2423:PHE:N	2.72	0.45
1:C:2127:LYS:HE2	1:C:2272:ILE:O	2.16	0.45
1:C:2416:TYR:HA	1:C:2429:ILE:HD13	1.98	0.44
1:A:350:TRP:CH2	1:A:393:ARG:HD3	2.52	0.44
1:B:1196:GLN:HA	1:B:1196:GLN:NE2	2.32	0.44
1:C:2358:TYR:CE2	1:C:2365:PRO:HG2	2.53	0.44
1:B:1120:GLU:HG2	2:B:5197:HOH:O	2.17	0.44
1:B:1173:PHE:CE2	1:B:1258:ILE:HD11	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2417:LEU:HD13	1:C:2417:LEU:C	2.42	0.44
1:A:334:ASP:O	1:A:338:LYS:HG3	2.18	0.44
1:A:324:LYS:N	1:A:324:LYS:HD2	2.33	0.44
1:A:451:LYS:O	1:A:452:ARG:HD3	2.18	0.44
1:D:3433:LYS:O	1:D:3434:ASP:HB2	2.18	0.44
1:C:2367:LEU:O	1:C:2371:GLU:HG3	2.18	0.44
1:A:124:LYS:NZ	2:A:4325:HOH:O	2.49	0.43
1:A:359:GLN:HB2	1:A:362:ASP:OD2	2.18	0.43
1:B:1291:LEU:HA	1:B:1295:GLN:HE21	1.83	0.43
1:D:3071:GLU:CD	1:D:3071:GLU:N	2.77	0.43
1:D:3353:MET:HE3	1:D:3358:TYR:CB	2.48	0.43
1:A:115:MET:HE3	1:A:393:ARG:NH1	2.32	0.43
1:B:1367:LEU:O	1:B:1371:GLU:HG3	2.19	0.43
1:C:2393:ARG:NH2	2:C:4848:HOH:O	2.51	0.43
1:D:3325:LEU:O	1:D:3329:ILE:HG13	2.19	0.43
1:B:1379:LYS:HD3	1:B:1437:TYR:OH	2.19	0.43
1:D:3197:VAL:HG11	1:D:3255:CYS:SG	2.58	0.43
1:A:166:ASN:HB3	1:A:169:ALA:CB	2.48	0.43
1:A:313:TYR:O	1:A:318:GLY:HA2	2.18	0.43
1:A:128:GLU:O	1:A:132:MET:HG3	2.19	0.43
1:B:1341:ILE:HA	1:B:1342:PRO:HD2	1.88	0.43
1:B:1363:PRO:HB3	1:D:3117:GLY:O	2.19	0.43
1:C:2353:MET:HE3	1:C:2358:TYR:CB	2.48	0.43
1:C:2424:ALA:C	1:C:2426:GLU:H	2.27	0.43
1:C:2444:GLU:HG2	1:C:2453:TYR:HE2	1.82	0.43
1:A:308:LYS:HB2	2:A:5170:HOH:O	2.19	0.42
1:B:1165:ILE:HG12	1:B:1254:GLU:HG2	2.00	0.42
1:C:2115:MET:HE3	1:C:2393:ARG:HH21	1.83	0.42
1:B:1108:TYR:CD2	1:B:1186:SER:HB3	2.54	0.42
1:D:3304:ARG:NH1	1:D:3304:ARG:CB	2.82	0.42
1:D:3319:GLY:O	1:D:3320:SER:C	2.62	0.42
1:C:2416:TYR:CZ	1:C:2418:SER:HB2	2.55	0.42
1:C:2418:SER:CB	1:C:2425:SER:HA	2.50	0.42
1:C:2450:VAL:CG1	1:C:2452:ARG:HH12	2.33	0.42
1:B:1197:VAL:HA	2:B:5192:HOH:O	2.19	0.42
1:B:1325:LEU:O	1:B:1329:ILE:HG13	2.20	0.42
1:B:1451:LYS:C	1:B:1452:ARG:HD2	2.44	0.42
1:D:3304:ARG:HH11	1:D:3304:ARG:CB	2.32	0.42
1:B:1361:SER:OG	1:D:3448:LYS:HE2	2.20	0.42
2:B:6775:HOH:O	1:C:2423:PHE:HE1	2.03	0.42
1:C:2423:PHE:CG	1:C:2424:ALA:N	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1115:MET:SD	1:B:1393:ARG:NH2	2.93	0.42
1:B:1295:GLN:HA	1:B:1331:ASN:HB3	2.00	0.42
1:C:2302:TYR:HD1	1:C:2310:ILE:HD12	1.84	0.42
1:C:2418:SER:HB3	1:C:2425:SER:HA	2.02	0.42
1:A:70:LYS:HD2	2:A:4005:HOH:O	2.19	0.42
1:D:3226:ASN:OD1	1:D:3227:ASN:ND2	2.53	0.42
1:C:2064:GLU:HG2	2:C:5287:HOH:O	2.19	0.41
1:D:3152:THR:HG21	2:D:4512:HOH:O	2.19	0.41
1:B:1277:HIS:HB3	2:B:4408:HOH:O	2.20	0.41
1:B:1286:GLU:HG2	1:B:1290:ASP:OD2	2.20	0.41
1:B:1302:TYR:HA	1:B:1306:ASP:HB2	2.03	0.41
1:C:2166:ASN:HB3	1:C:2169:ALA:CB	2.50	0.41
1:A:304:ARG:HG2	1:A:305:GLN:OE1	2.21	0.41
1:A:314:LEU:HD21	1:A:329:ILE:HD13	2.03	0.41
1:C:2174:LYS:HD2	1:C:2245:VAL:HB	2.02	0.41
1:C:2360:ILE:HD12	1:C:2360:ILE:C	2.46	0.41
1:A:353:MET:HE3	1:A:358:TYR:HB2	2.02	0.41
1:A:393:ARG:HH11	1:A:398:GLY:HA3	1.85	0.41
1:C:2385:MET:HE3	1:C:2431:LEU:CD1	2.40	0.41
1:D:3076:TRP:CE2	1:D:3080:LYS:NZ	2.85	0.41
1:D:3400:ARG:HG3	1:D:3400:ARG:NH1	2.36	0.41
1:B:1070:LYS:HD3	2:B:6803:HOH:O	2.19	0.41
1:D:3317:GLN:HG2	1:D:3320:SER:HB3	2.02	0.41
1:D:3326:ASP:N	2:D:6997:HOH:O	2.52	0.41
1:D:3426:GLU:CD	1:D:3426:GLU:N	2.79	0.41
1:A:197:VAL:HG12	1:A:198:SER:O	2.21	0.41
1:A:296:ARG:O	1:A:300:ASP:OD2	2.38	0.41
1:D:3318:GLY:C	1:D:3320:SER:N	2.79	0.41
1:B:1378:ILE:CD1	1:B:1460:LEU:HD11	2.35	0.41
1:C:2101:LYS:HG3	1:C:2102:ASN:ND2	2.36	0.41
1:C:2115:MET:HE3	1:C:2393:ARG:CZ	2.50	0.41
1:C:2186:SER:HB2	2:C:5914:HOH:O	2.21	0.41
1:C:2358:TYR:CZ	1:C:2365:PRO:HG2	2.56	0.41
1:D:3307:TYR:CD1	1:D:3308:LYS:N	2.89	0.41
1:A:71:GLU:N	1:A:71:GLU:CD	2.79	0.40
1:C:2128:GLU:O	1:C:2132:MET:HG3	2.21	0.40
1:C:2433:LYS:O	1:C:2434:ASP:HB2	2.21	0.40
1:A:448:LYS:HE2	2:A:4336:HOH:O	2.20	0.40
1:B:1322:ASN:C	1:B:1322:ASN:ND2	2.78	0.40
1:A:416:TYR:CE2	1:A:418:SER:HB2	2.57	0.40
1:D:3302:TYR:HA	1:D:3306:ASP:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:GLU:CD	1:A:71:GLU:H	2.30	0.40
1:C:2353:MET:HE3	1:C:2358:TYR:HB2	2.02	0.40
1:B:1149:GLU:CD	1:B:1150:PRO:HD2	2.47	0.40
1:B:1174:LYS:HD3	2:B:6165:HOH:O	2.21	0.40
1:C:2306:ASP:O	1:C:2310:ILE:HG13	2.22	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	400/462 (87%)	391 (98%)	7 (2%)	2 (0%)	24	8
1	B	400/462 (87%)	386 (96%)	9 (2%)	5 (1%)	9	1
1	C	400/462 (87%)	380 (95%)	13 (3%)	7 (2%)	6	1
1	D	400/462 (87%)	384 (96%)	10 (2%)	6 (2%)	8	1
All	All	1600/1848 (87%)	1541 (96%)	39 (2%)	20 (1%)	9	1

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1320	SER
1	D	3320	SER
1	D	3424	ALA
1	D	3425	SER
1	B	1318	GLY
1	B	1425	SER
1	C	2305	GLN
1	C	2423	PHE
1	A	322	ASN
1	B	1199	SER

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Mol	Chain	Res	Type
1	B	1304	ARG
1	C	2198	SER
1	C	2200	LYS
1	C	2322	ASN
1	C	2425	SER
1	D	3322	ASN
1	A	305	GLN
1	D	3305	GLN
1	C	2321	GLY
1	D	3323	GLU

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	356/414 (86%)	356 (100%)	0	100	100
1	B	356/414 (86%)	353 (99%)	3 (1%)	73	54
1	C	356/414 (86%)	356 (100%)	0	100	100
1	D	356/414 (86%)	354 (99%)	2 (1%)	78	62
All	All	1424/1656 (86%)	1419 (100%)	5 (0%)	84	71

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1070	LYS
1	B	1200	LYS
1	B	1305	GLN
1	D	3072	LYS
1	D	3436	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	ASN

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Mol	Chain	Res	Type
1	A	107	ASN
1	A	172	GLN
1	A	227	ASN
1	A	331	ASN
1	A	373	GLN
1	A	438	HIS
1	B	1096	ASN
1	B	1107	ASN
1	B	1196	GLN
1	B	1227	ASN
1	B	1236	ASN
1	B	1295	GLN
1	B	1305	GLN
1	B	1322	ASN
1	B	1328	GLN
1	B	1376	ASN
1	C	2096	ASN
1	C	2102	ASN
1	C	2107	ASN
1	C	2137	ASN
1	C	2140	ASN
1	C	2147	ASN
1	C	2156	ASN
1	C	2227	ASN
1	C	2312	ASN
1	C	2316	ASN
1	C	2359	GLN
1	C	2376	ASN
1	D	3096	ASN
1	D	3107	ASN
1	D	3137	ASN
1	D	3140	ASN
1	D	3227	ASN
1	D	3283	ASN
1	D	3312	ASN
1	D	3316	ASN
1	D	3373	GLN
1	D	3376	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.