



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:08 AM UTC

PDB ID : 1S9H / pdb_00001s9h
Title : Crystal Structure of Adeno-associated virus Type 2 Rep40
Authors : James, J.A.; Escalante, C.R.; Yoon-Robarts, M.; Edwards, T.A.; Linden, R.M.; Aggarwal, A.K.
Deposited on : 2004-02-04
Resolution : 2.40 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

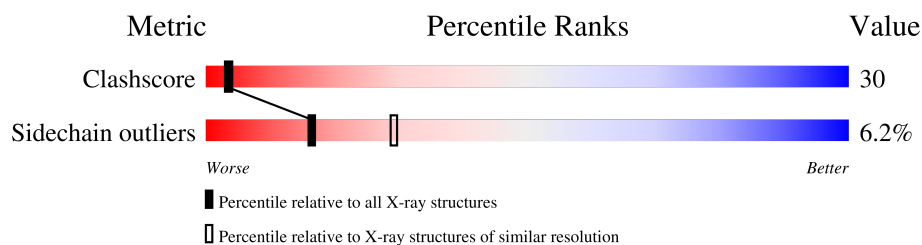
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	5391 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

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	268	54% 40% 6%
1	B	268	60% 36% .
1	C	268	38% 33% . 26%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5963 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 Rep 40 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	0	0
			2080	1329	350	391	10			
1	B	267	Total	C	N	O	S	0	0	0
			2064	1319	346	389	10			
1	C	199	Total	C	N	O	S	0	0	0
			1462	947	240	270	5			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	223	ALA	-	cloning artifact	GB 2906019
A	224	GLY	-	cloning artifact	GB 2906019
B	223	ALA	-	cloning artifact	GB 2906019
B	224	GLY	-	cloning artifact	GB 2906019
C	223	ALA	-	cloning artifact	GB 2906019
C	224	GLY	-	cloning artifact	GB 2906019

- Molecule 2 is water.

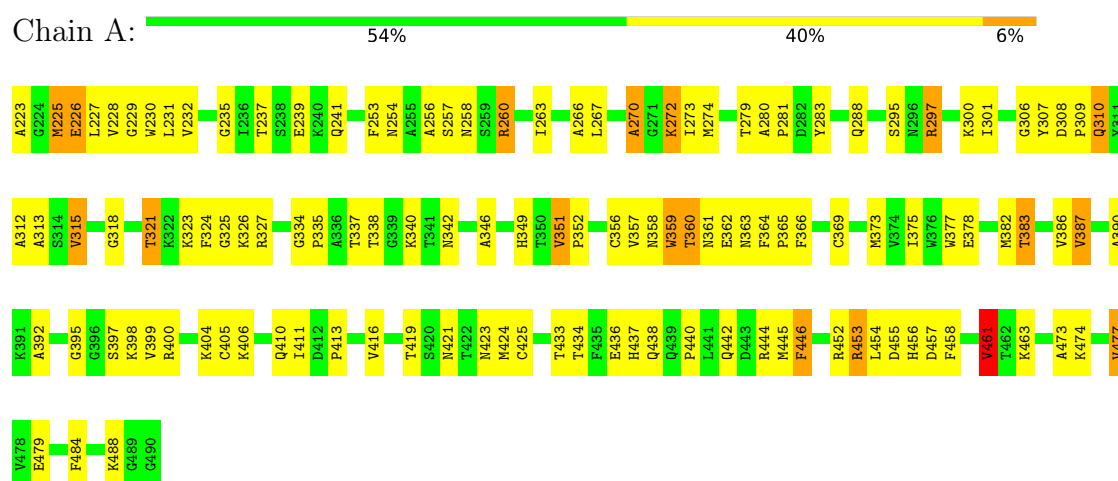
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	166	Total	O	0	0
			166	166		
2	B	117	Total	O	0	0
			117	117		
2	C	74	Total	O	0	0
			74	74		

3 Residue-property plots

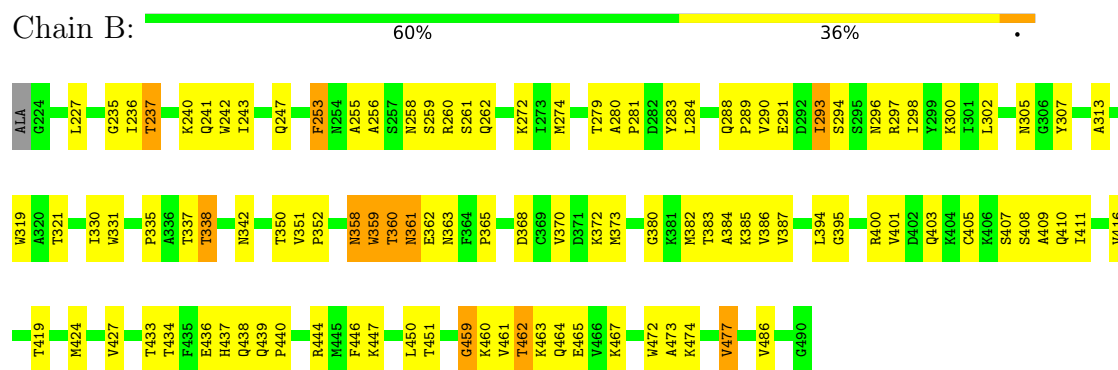
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

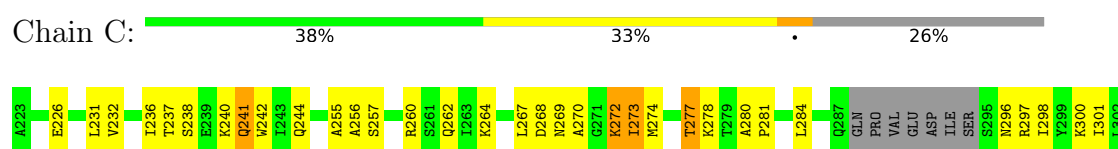
• Molecule 1: Rep 40 protein

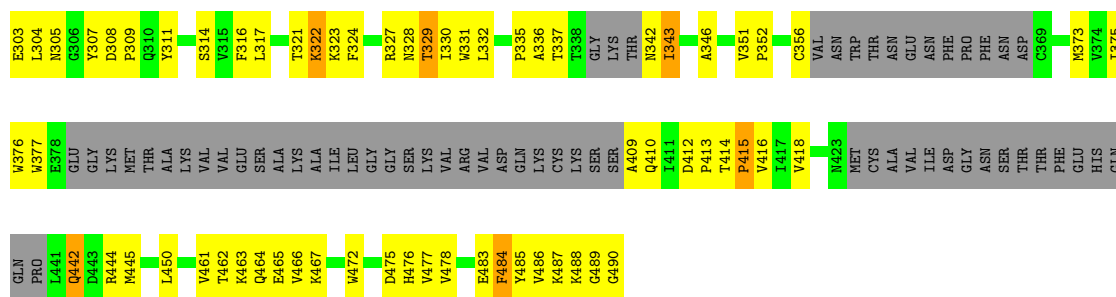


• Molecule 1: Rep 40 protein



• Molecule 1: Rep 40 protein





4 Data and refinement statistics

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

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	126.29Å 126.29Å 97.89Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.97 – 2.40	Depositor
% Data completeness (in resolution range)	85.5 (19.97-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.227 , 0.293	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5963	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

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	0.51	0/2130	1.09	19/2890 (0.7%)
1	B	0.46	0/2113	0.96	9/2868 (0.3%)
1	C	0.40	0/1494	1.01	12/2033 (0.6%)
All	All	0.47	0/5737	1.02	40/7791 (0.5%)

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	262	GLN	OE1-CD-NE2	-9.84	112.76	122.60
1	A	288	GLN	OE1-CD-NE2	-9.84	112.76	122.60
1	A	310	GLN	OE1-CD-NE2	-9.82	112.78	122.60
1	C	241	GLN	OE1-CD-NE2	-9.78	112.82	122.60
1	A	410	GLN	OE1-CD-NE2	-9.76	112.84	122.60
1	A	270	ALA	N-CA-C	-9.53	97.95	110.53
1	A	360	THR	N-CA-C	-8.57	101.43	112.23
1	A	272	LYS	N-CA-C	-8.57	101.89	111.14
1	C	351	VAL	CA-C-N	6.70	126.21	119.24
1	C	351	VAL	C-N-CA	6.70	126.21	119.24
1	A	310	GLN	CG-CD-NE2	6.68	126.42	116.40
1	C	241	GLN	CG-CD-NE2	6.68	126.42	116.40
1	C	262	GLN	CG-CD-NE2	6.67	126.41	116.40
1	A	288	GLN	CG-CD-NE2	6.66	126.39	116.40
1	A	410	GLN	CG-CD-NE2	6.66	126.39	116.40
1	C	226	GLU	N-CA-C	-6.63	105.01	113.23
1	A	477	VAL	N-CA-C	6.43	117.33	108.84
1	C	296	ASN	N-CA-C	6.41	117.59	108.74
1	B	459	GLY	N-CA-C	6.28	118.44	110.96
1	C	335	PRO	N-CA-CB	6.27	109.83	103.25
1	A	446	PHE	N-CA-C	-6.05	98.55	108.41
1	B	351	VAL	CA-C-N	5.99	125.20	118.97
1	B	351	VAL	C-N-CA	5.99	125.20	118.97
1	B	477	VAL	N-CA-C	5.96	116.71	108.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	226	GLU	N-CA-C	-5.89	105.94	113.01
1	B	359	TRP	N-CA-C	-5.89	105.91	112.57
1	B	446	PHE	N-CA-C	-5.83	98.91	108.41
1	B	358	ASN	N-CA-C	-5.81	100.67	109.85
1	A	387	VAL	N-CA-C	5.68	117.09	110.62
1	C	484	PHE	N-CA-C	-5.48	102.17	110.28
1	A	458	PHE	N-CA-C	-5.47	105.40	111.36
1	A	461	VAL	N-CA-C	-5.33	102.70	109.58
1	A	438	GLN	N-CA-C	5.33	117.51	111.11
1	C	323	LYS	N-CA-C	5.32	122.14	110.80
1	B	438	GLN	N-CA-C	5.32	117.50	111.11
1	C	343	ILE	N-CA-C	-5.30	105.96	111.58
1	B	360	THR	N-CA-C	-5.24	106.73	113.01
1	A	378	GLU	N-CA-C	5.18	118.75	112.23
1	A	421	ASN	N-CA-C	-5.14	105.90	113.61
1	A	369	CYS	N-CA-C	5.02	119.36	112.88

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	2080	0	2003	123	0
1	B	2064	0	1969	106	0
1	C	1462	0	1314	100	0
2	A	166	0	0	13	0
2	B	117	0	0	2	0
2	C	74	0	0	3	0
All	All	5963	0	5286	326	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 30.

All (326) 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:434:THR:HG22	1:A:436:GLU:H	1.20	1.05
1:B:293:ILE:H	1:B:293:ILE:HD12	1.21	1.01
1:C:238:SER:OG	1:C:241:GLN:HG2	1.65	0.95
1:A:453:ARG:H	1:A:453:ARG:HE	1.17	0.88
1:C:307:TYR:O	1:C:309:PRO:HD3	1.72	0.88
1:B:342:ASN:HD21	1:B:460:LYS:H	1.23	0.86
1:A:357:VAL:HG12	1:A:377:TRP:HA	1.60	0.83
1:A:357:VAL:CG1	1:A:377:TRP:HA	2.08	0.82
1:C:322:LYS:HA	1:C:322:LYS:NZ	1.94	0.81
1:C:297:ARG:HG2	1:C:461:VAL:HA	1.62	0.81
1:B:280:ALA:HA	1:B:373:MET:HE3	1.64	0.79
1:B:459:GLY:O	1:B:460:LYS:HB2	1.83	0.79
1:A:359:TRP:CZ2	1:A:382:MET:HA	2.17	0.78
1:A:392:ALA:HB3	1:A:399:VAL:HG21	1.66	0.78
1:A:337:THR:O	1:A:337:THR:HG22	1.82	0.78
1:A:392:ALA:CB	1:A:399:VAL:HG21	2.14	0.78
1:C:322:LYS:HA	1:C:322:LYS:HZ3	1.48	0.77
1:B:305:ASN:ND2	1:B:451:THR:H	1.84	0.76
1:B:305:ASN:HD21	1:B:451:THR:H	1.32	0.76
1:B:462:THR:HG22	1:B:465:GLU:HG3	1.68	0.76
1:B:462:THR:CG2	1:B:465:GLU:H	1.99	0.75
1:C:463:LYS:HD3	1:C:463:LYS:N	2.02	0.75
1:C:305:ASN:HB3	1:C:488:LYS:HZ3	1.52	0.74
1:A:231:LEU:N	2:A:496:HOH:O	2.20	0.74
1:A:334:GLY:O	1:A:340:LYS:HE2	1.88	0.74
1:A:228:VAL:O	2:A:496:HOH:O	2.06	0.74
1:C:269:ASN:O	1:C:273:ILE:HG23	1.88	0.74
1:B:338:THR:HG21	1:B:450:LEU:C	2.13	0.73
1:A:279:THR:HG22	1:A:280:ALA:N	2.04	0.72
1:C:273:ILE:O	1:C:277:THR:HB	1.90	0.72
1:B:305:ASN:ND2	1:B:450:LEU:HA	2.04	0.72
1:C:321:THR:HG22	1:C:322:LYS:H	1.54	0.71
1:C:375:ILE:HB	1:C:416:VAL:HG22	1.71	0.71
1:B:361:ASN:C	1:B:361:ASN:HD22	1.97	0.71
1:C:305:ASN:HB3	1:C:488:LYS:NZ	2.05	0.71
1:A:453:ARG:H	1:A:453:ARG:NE	1.89	0.70
1:C:342:ASN:OD1	1:C:461:VAL:HG23	1.90	0.70
1:B:294:SER:O	1:B:300:LYS:HE3	1.91	0.69
1:A:404:LYS:NZ	1:B:405:CYS:HB3	2.08	0.69
1:A:327:ARG:HD2	1:A:445:MET:O	1.93	0.68
1:C:463:LYS:HD3	1:C:463:LYS:H	1.58	0.68
1:A:392:ALA:HB1	1:A:399:VAL:CG2	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:ASN:HB3	1:B:360:THR:HG23	1.76	0.68
1:B:279:THR:HG22	1:B:281:PRO:CD	2.24	0.68
1:C:280:ALA:HB3	1:C:281:PRO:HD3	1.76	0.67
1:B:403:GLN:HB2	1:B:407:SER:CB	2.24	0.67
1:A:357:VAL:HG11	1:A:377:TRP:CG	2.29	0.67
1:B:462:THR:HG23	1:B:465:GLU:H	1.59	0.67
1:B:359:TRP:CD1	1:B:380:GLY:HA3	2.29	0.67
1:A:325:GLY:O	1:A:326:LYS:HB2	1.93	0.67
1:A:232:VAL:HG22	2:A:491:HOH:O	1.95	0.66
1:A:312:ALA:O	1:A:315:VAL:HG13	1.96	0.66
1:B:290:VAL:O	1:B:291:GLU:HB3	1.94	0.66
1:B:261:SER:O	1:B:262:GLN:HB2	1.95	0.66
1:C:414:THR:O	1:C:416:VAL:HG23	1.97	0.65
1:A:229:GLY:C	2:A:496:HOH:O	2.40	0.64
1:A:377:TRP:CZ2	1:A:424:MET:HE1	2.31	0.64
1:B:293:ILE:H	1:B:293:ILE:CD1	1.96	0.64
1:B:382:MET:CE	1:B:387:VAL:HA	2.28	0.64
1:A:335:PRO:O	1:A:338:THR:HG22	1.96	0.64
1:A:352:PRO:HD2	1:A:373:MET:SD	2.37	0.64
1:A:382:MET:CE	1:A:387:VAL:HG23	2.26	0.64
1:B:321:THR:O	1:B:321:THR:HG22	1.96	0.64
1:C:308:ASP:HB2	1:C:490:GLY:HA2	1.80	0.64
1:B:384:ALA:HA	1:B:387:VAL:CG2	2.28	0.64
1:A:375:ILE:HB	1:A:416:VAL:HG22	1.79	0.64
1:B:462:THR:HG22	1:B:465:GLU:CG	2.27	0.63
1:A:297:ARG:CG	1:A:297:ARG:HH11	2.11	0.63
1:C:332:LEU:HD22	1:C:450:LEU:HD11	1.81	0.63
1:B:279:THR:HG22	1:B:281:PRO:HD2	1.82	0.62
1:B:439:GLN:HB3	1:B:440:PRO:HD3	1.82	0.62
1:B:382:MET:HE3	1:B:387:VAL:HA	1.81	0.62
1:C:475:ASP:C	1:C:476:HIS:ND1	2.58	0.62
1:A:357:VAL:HG11	1:A:377:TRP:CD1	2.34	0.62
1:A:404:LYS:HZ3	1:B:405:CYS:HB3	1.64	0.61
1:C:442:GLN:OE1	1:C:442:GLN:HA	2.00	0.61
1:B:280:ALA:CA	1:B:373:MET:HE3	2.29	0.61
1:B:342:ASN:ND2	1:B:460:LYS:H	1.92	0.61
1:B:236:ILE:HD13	1:B:242:TRP:HA	1.83	0.61
1:A:254:ASN:HD21	1:A:263:ILE:HD11	1.66	0.60
1:B:305:ASN:HD21	1:B:451:THR:N	1.99	0.60
1:B:474:LYS:O	1:B:477:VAL:HG23	2.01	0.60
1:B:437:HIS:O	1:B:440:PRO:HD2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:317:LEU:HD23	1:C:317:LEU:C	2.26	0.60
1:C:332:LEU:HB3	1:C:450:LEU:HD13	1.82	0.60
1:A:279:THR:HG22	1:A:281:PRO:CD	2.32	0.60
1:B:447:LYS:O	1:B:486:VAL:HG23	2.02	0.60
1:A:392:ALA:CB	1:A:399:VAL:CG2	2.77	0.60
1:C:232:VAL:HG21	1:C:273:ILE:CD1	2.32	0.60
1:C:356:CYS:CB	1:C:376:TRP:HB3	2.31	0.60
1:A:337:THR:O	1:A:337:THR:CG2	2.50	0.60
1:B:313:ALA:HB1	1:B:473:ALA:HB2	1.84	0.59
1:A:382:MET:HE1	1:A:387:VAL:HG23	1.84	0.59
1:B:280:ALA:HA	1:B:373:MET:CE	2.32	0.59
1:B:279:THR:HG22	1:B:280:ALA:N	2.18	0.59
1:C:321:THR:HG22	1:C:322:LYS:N	2.18	0.59
1:B:293:ILE:HG12	1:B:472:TRP:CD1	2.38	0.58
1:B:434:THR:HG22	1:B:436:GLU:H	1.68	0.58
1:A:307:TYR:O	1:A:309:PRO:HD3	2.03	0.58
1:A:411:ILE:HB	2:A:497:HOH:O	2.03	0.58
1:B:280:ALA:N	1:B:373:MET:HE3	2.18	0.58
1:A:357:VAL:O	1:A:357:VAL:HG13	2.03	0.58
1:B:255:ALA:O	1:B:256:ALA:HB3	2.04	0.58
1:B:227:LEU:HD22	1:B:253:PHE:CE2	2.38	0.58
1:C:277:THR:HG22	1:C:278:LYS:HD2	1.85	0.58
1:A:279:THR:HG22	1:A:281:PRO:HD2	1.85	0.57
1:B:279:THR:HG22	1:B:281:PRO:HD3	1.85	0.57
1:B:298:ILE:O	1:B:302:LEU:HD13	2.04	0.57
1:C:304:LEU:HD12	1:C:305:ASN:HB2	1.87	0.57
1:B:370:VAL:O	1:B:372:LYS:HE2	2.04	0.57
1:C:484:PHE:O	1:C:485:TYR:HB2	2.05	0.57
1:B:272:LYS:HE2	1:B:272:LYS:HA	1.87	0.56
1:A:239:GLU:CD	1:A:260:ARG:HH22	2.14	0.56
1:A:325:GLY:O	1:A:326:LYS:CB	2.54	0.56
1:A:279:THR:HG22	1:A:280:ALA:H	1.68	0.56
1:C:278:LYS:HB3	1:C:373:MET:HE1	1.88	0.56
1:A:232:VAL:N	2:A:496:HOH:O	2.01	0.56
1:A:223:ALA:HB3	1:A:226:GLU:CB	2.36	0.56
1:A:237:THR:H	1:A:241:GLN:NE2	2.04	0.56
1:A:254:ASN:ND2	1:A:263:ILE:HD11	2.20	0.56
1:C:297:ARG:C	1:C:301:ILE:HG12	2.31	0.56
1:A:321:THR:HG22	1:A:323:LYS:HB2	1.88	0.55
1:A:437:HIS:O	1:A:440:PRO:HD2	2.06	0.55
1:B:290:VAL:O	1:B:291:GLU:CB	2.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:462:THR:CG2	1:B:464:GLN:HB3	2.37	0.55
1:A:231:LEU:HD13	1:A:267:LEU:HD23	1.89	0.55
1:B:462:THR:CG2	1:B:465:GLU:HG3	2.35	0.55
1:A:349:HIS:HB2	1:A:463:LYS:HE3	1.89	0.55
1:A:279:THR:CG2	1:A:280:ALA:N	2.70	0.54
1:C:304:LEU:HD12	1:C:305:ASN:N	2.23	0.54
1:B:237:THR:HB	1:B:241:GLN:OE1	2.07	0.54
1:C:329:THR:HA	1:C:416:VAL:O	2.07	0.54
1:C:346:ALA:O	1:C:466:VAL:HG21	2.08	0.54
1:C:304:LEU:HD12	1:C:305:ASN:CB	2.38	0.54
1:A:437:HIS:C	1:A:440:PRO:HD2	2.32	0.54
1:A:423:ASN:ND2	1:A:425:CYS:H	2.05	0.54
1:B:382:MET:HE1	1:B:387:VAL:HG13	1.90	0.53
1:A:297:ARG:HH11	1:A:297:ARG:HG2	1.73	0.53
1:C:300:LYS:HG3	2:C:524:HOH:O	2.08	0.53
1:A:280:ALA:HB3	1:A:281:PRO:HD3	1.89	0.53
1:B:462:THR:HG23	1:B:464:GLN:N	2.24	0.53
1:A:256:ALA:O	1:A:257:SER:CB	2.56	0.53
1:B:335:PRO:HD2	1:B:450:LEU:O	2.09	0.53
1:A:398:LYS:HG3	2:B:514:HOH:O	2.09	0.53
1:B:462:THR:HG22	1:B:465:GLU:H	1.71	0.53
1:C:327:ARG:O	1:C:328:ASN:C	2.52	0.53
1:C:336:ALA:O	1:C:337:THR:CB	2.57	0.53
1:C:375:ILE:O	1:C:416:VAL:HA	2.08	0.53
1:C:463:LYS:H	1:C:463:LYS:CD	2.21	0.53
1:B:395:GLY:HA3	1:B:444:ARG:HH11	1.73	0.53
1:C:311:TYR:CE2	1:C:487:LYS:HB2	2.45	0.52
1:B:319:TRP:CD1	1:B:330:ILE:HG13	2.44	0.52
1:B:335:PRO:HB2	1:B:338:THR:OG1	2.09	0.52
1:A:361:ASN:O	1:A:363:ASN:N	2.42	0.52
1:C:304:LEU:O	1:C:305:ASN:C	2.53	0.52
1:A:225:MET:HG3	1:A:228:VAL:HG23	1.91	0.52
1:B:302:LEU:O	1:B:307:TYR:HB2	2.09	0.52
1:C:303:GLU:OE1	1:C:303:GLU:HA	2.10	0.52
1:A:297:ARG:O	1:A:301:ILE:HG22	2.09	0.52
1:C:297:ARG:O	1:C:298:ILE:C	2.52	0.52
1:A:377:TRP:CE2	1:A:424:MET:HE1	2.45	0.52
1:B:352:PRO:HD2	1:B:373:MET:CE	2.40	0.51
1:C:297:ARG:O	1:C:300:LYS:N	2.43	0.51
1:B:227:LEU:HD22	1:B:253:PHE:CZ	2.45	0.51
1:B:297:ARG:HG3	1:B:465:GLU:OE2	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:346:ALA:CB	1:C:461:VAL:HB	2.41	0.51
1:C:297:ARG:HD3	1:C:465:GLU:OE1	2.10	0.51
1:C:232:VAL:HG21	1:C:273:ILE:HD11	1.91	0.51
1:C:307:TYR:CD2	1:C:488:LYS:HA	2.46	0.51
1:C:415:PRO:O	1:C:416:VAL:HB	2.11	0.51
1:B:400:ARG:HH11	1:B:400:ARG:HG2	1.75	0.51
1:C:450:LEU:HD12	1:C:450:LEU:N	2.27	0.50
1:A:434:THR:HG22	1:A:436:GLU:N	2.06	0.50
1:C:304:LEU:HD11	1:C:450:LEU:HA	1.94	0.50
1:B:293:ILE:HD12	1:B:293:ILE:N	2.06	0.50
1:A:382:MET:HE3	1:A:390:ALA:HB3	1.93	0.50
1:C:461:VAL:O	1:C:462:THR:HB	2.11	0.50
1:A:279:THR:CG2	1:A:280:ALA:H	2.25	0.50
1:A:342:ASN:ND2	1:A:461:VAL:HG13	2.27	0.50
1:A:442:GLN:HG2	1:A:484:PHE:CZ	2.47	0.50
1:C:377:TRP:CE3	1:C:418:VAL:HG22	2.47	0.50
1:B:283:TYR:HD1	1:B:373:MET:HE1	1.77	0.49
1:B:400:ARG:HA	1:B:409:ALA:O	2.12	0.49
1:B:368:ASP:O	1:B:372:LYS:HE3	2.11	0.49
1:C:311:TYR:CZ	1:C:487:LYS:HD3	2.47	0.49
1:C:316:PHE:CE2	1:C:330:ILE:HD12	2.47	0.49
1:A:313:ALA:HB1	1:A:473:ALA:HB2	1.94	0.49
1:A:346:ALA:CB	1:A:461:VAL:HG22	2.42	0.49
1:B:363:ASN:O	1:B:365:PRO:HD3	2.12	0.49
1:A:223:ALA:HB3	1:A:226:GLU:HB3	1.95	0.49
1:A:395:GLY:HA3	1:A:444:ARG:HD3	1.93	0.49
1:B:342:ASN:HD21	1:B:460:LYS:N	2.03	0.49
1:A:273:ILE:HB	2:A:491:HOH:O	2.11	0.49
1:A:295:SER:HA	1:A:300:LYS:NZ	2.27	0.49
1:B:361:ASN:C	1:B:361:ASN:ND2	2.68	0.49
1:C:463:LYS:N	1:C:463:LYS:CD	2.74	0.49
1:A:358:ASN:O	1:A:359:TRP:HB2	2.12	0.49
1:A:366:PHE:HE1	1:A:386:VAL:HG13	1.78	0.49
1:A:405:CYS:O	1:A:406:LYS:C	2.56	0.49
1:A:452:ARG:HA	1:A:453:ARG:HH21	1.76	0.48
1:B:437:HIS:C	1:B:440:PRO:HD2	2.38	0.48
1:C:297:ARG:HD2	1:C:297:ARG:N	2.28	0.48
1:A:363:ASN:C	1:A:365:PRO:HD3	2.38	0.48
1:A:453:ARG:HE	1:A:453:ARG:N	1.97	0.48
1:C:255:ALA:O	1:C:256:ALA:HB3	2.14	0.48
1:C:328:ASN:O	1:C:329:THR:HG23	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:444:ARG:O	1:C:445:MET:HB3	2.13	0.48
1:C:487:LYS:C	1:C:489:GLY:H	2.20	0.48
1:B:243:ILE:HG23	1:B:247:GLN:HG3	1.95	0.48
1:A:398:LYS:HG2	1:A:413:PRO:HD3	1.95	0.48
1:B:462:THR:HG23	1:B:464:GLN:HB3	1.94	0.48
1:C:328:ASN:HB3	1:C:415:PRO:O	2.13	0.48
1:B:331:TRP:CH2	1:B:424:MET:HB2	2.49	0.48
1:B:258:ASN:C	1:B:260:ARG:H	2.22	0.47
1:C:297:ARG:HD2	1:C:297:ARG:H	1.79	0.47
1:A:452:ARG:HG2	2:A:564:HOH:O	2.14	0.47
1:A:473:ALA:O	1:A:477:VAL:HG22	2.15	0.47
1:B:350:THR:HA	1:B:463:LYS:HE3	1.96	0.47
1:A:395:GLY:CA	1:A:444:ARG:HD3	2.45	0.47
1:C:352:PRO:HD2	1:C:373:MET:SD	2.54	0.47
1:A:267:LEU:O	1:A:270:ALA:O	2.33	0.47
1:C:484:PHE:O	1:C:485:TYR:CB	2.63	0.47
1:A:235:GLY:HA2	1:A:274:MET:SD	2.54	0.47
1:A:297:ARG:CG	1:A:297:ARG:NH1	2.75	0.47
1:C:278:LYS:HB3	1:C:373:MET:CE	2.45	0.47
1:A:301:ILE:HB	2:A:495:HOH:O	2.13	0.47
1:A:306:GLY:O	1:A:488:LYS:HB3	2.15	0.47
1:B:427:VAL:O	1:B:433:THR:HG23	2.14	0.47
1:A:324:PHE:O	1:A:325:GLY:C	2.57	0.46
1:A:361:ASN:C	1:A:363:ASN:N	2.72	0.46
1:B:284:LEU:O	1:B:467:LYS:HA	2.14	0.46
1:C:240:LYS:O	1:C:244:GLN:HG3	2.15	0.46
1:A:423:ASN:HD22	1:A:424:MET:N	2.14	0.46
1:A:454:LEU:O	1:A:455:ASP:HB2	2.15	0.46
1:C:255:ALA:C	1:C:257:SER:H	2.22	0.46
1:A:457:ASP:OD2	1:A:457:ASP:C	2.59	0.46
1:C:331:TRP:HA	1:C:418:VAL:O	2.15	0.46
1:A:295:SER:HA	1:A:300:LYS:HZ3	1.80	0.46
1:C:487:LYS:O	1:C:489:GLY:N	2.47	0.45
1:A:237:THR:H	1:A:241:GLN:HE22	1.65	0.45
1:C:236:ILE:HD13	1:C:242:TRP:HA	1.99	0.45
1:A:239:GLU:OE2	1:A:260:ARG:NH2	2.49	0.45
1:C:373:MET:O	1:C:415:PRO:HD2	2.16	0.45
1:C:413:PRO:HG2	2:C:548:HOH:O	2.16	0.45
1:B:401:VAL:O	1:B:408:SER:HA	2.16	0.45
1:C:322:LYS:O	1:C:324:PHE:N	2.50	0.45
1:C:377:TRP:HE3	1:C:418:VAL:HG22	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:256:ALA:O	1:C:257:SER:HB2	2.17	0.45
1:B:400:ARG:NH2	1:B:408:SER:OG	2.50	0.45
1:A:227:LEU:HD13	1:A:253:PHE:CD2	2.52	0.44
1:B:279:THR:CG2	1:B:281:PRO:HD2	2.46	0.44
1:B:337:THR:HG21	2:B:579:HOH:O	2.17	0.44
1:B:434:THR:CG2	1:B:436:GLU:HG2	2.47	0.44
1:A:321:THR:O	1:A:321:THR:CG2	2.66	0.44
1:A:279:THR:HG22	1:A:281:PRO:HD3	1.99	0.44
1:C:472:TRP:NE1	1:C:476:HIS:NE2	2.66	0.44
1:A:230:TRP:C	2:A:496:HOH:O	2.59	0.44
1:A:404:LYS:HA	1:A:404:LYS:HD3	1.76	0.44
1:A:423:ASN:HD22	1:A:423:ASN:C	2.24	0.44
1:C:238:SER:HB2	2:C:493:HOH:O	2.17	0.44
1:A:258:ASN:OD1	1:A:260:ARG:NH1	2.51	0.43
1:A:382:MET:HE3	1:A:390:ALA:CB	2.48	0.43
1:A:327:ARG:HG2	1:A:446:PHE:CE1	2.53	0.43
1:A:474:LYS:O	1:A:477:VAL:HG23	2.18	0.43
1:B:279:THR:C	1:B:373:MET:HE3	2.42	0.43
1:A:404:LYS:HZ2	1:B:405:CYS:HB3	1.82	0.43
1:A:256:ALA:O	1:A:257:SER:HB3	2.17	0.43
1:A:362:GLU:OE1	1:A:383:THR:HG21	2.19	0.43
1:B:296:ASN:O	1:B:300:LYS:HG3	2.18	0.43
1:C:322:LYS:HA	1:C:322:LYS:HZ2	1.80	0.43
1:C:331:TRP:CD1	1:C:332:LEU:N	2.87	0.43
1:B:460:LYS:O	1:B:461:VAL:O	2.36	0.43
1:C:343:ILE:HA	1:C:461:VAL:HG21	2.01	0.43
1:A:225:MET:HE2	1:A:266:ALA:HB2	2.01	0.43
1:B:383:THR:CG2	1:B:386:VAL:HG22	2.48	0.43
1:C:346:ALA:HB2	1:C:461:VAL:HB	2.00	0.42
1:B:279:THR:CG2	1:B:280:ALA:N	2.82	0.42
1:A:442:GLN:HG2	1:A:484:PHE:CE1	2.54	0.42
1:B:394:LEU:HD23	1:B:416:VAL:HG11	2.01	0.42
1:C:304:LEU:HD12	1:C:304:LEU:C	2.44	0.42
1:A:283:TYR:CE1	1:A:373:MET:HE1	2.54	0.42
1:C:231:LEU:HD13	1:C:267:LEU:HD23	2.01	0.42
1:C:314:SER:OG	1:C:477:VAL:HA	2.19	0.42
1:A:274:MET:HG3	2:A:491:HOH:O	2.19	0.42
1:C:241:GLN:HA	1:C:241:GLN:OE1	2.20	0.42
1:C:284:LEU:O	1:C:467:LYS:HA	2.20	0.42
1:C:486:VAL:O	1:C:488:LYS:N	2.53	0.42
1:A:456:HIS:O	1:A:457:ASP:CG	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:260:ARG:NE	1:C:260:ARG:HA	2.34	0.42
1:A:279:THR:CG2	1:A:281:PRO:HD2	2.48	0.42
1:C:268:ASP:O	1:C:272:LYS:HB2	2.19	0.42
1:C:409:ALA:O	1:C:410:GLN:CB	2.68	0.42
1:C:487:LYS:O	1:C:488:LYS:HB3	2.19	0.42
1:C:324:PHE:HB2	1:C:327:ARG:CB	2.50	0.41
1:C:462:THR:HG22	1:C:464:GLN:H	1.84	0.41
1:A:308:ASP:OD1	1:A:308:ASP:C	2.62	0.41
1:A:361:ASN:C	1:A:363:ASN:H	2.28	0.41
1:B:294:SER:O	1:B:300:LYS:CE	2.64	0.41
1:C:300:LYS:HA	1:C:303:GLU:HG2	2.01	0.41
1:B:352:PRO:HD2	1:B:373:MET:HE2	2.01	0.41
1:B:255:ALA:O	1:B:256:ALA:CB	2.67	0.41
1:B:386:VAL:O	1:B:386:VAL:HG23	2.19	0.41
1:A:318:GLY:HA3	1:A:324:PHE:CE1	2.55	0.41
1:A:399:VAL:HG12	1:A:400:ARG:N	2.36	0.41
1:B:400:ARG:NH1	1:B:410:GLN:HG2	2.36	0.41
1:B:462:THR:HG21	1:B:464:GLN:HB3	2.01	0.41
1:A:351:VAL:HG22	1:A:352:PRO:HD2	2.03	0.41
1:B:235:GLY:HA2	1:B:274:MET:SD	2.61	0.41
1:C:270:ALA:O	1:C:274:MET:HG3	2.21	0.41
1:A:274:MET:N	2:A:491:HOH:O	2.54	0.41
1:A:397:SER:O	1:A:399:VAL:HG23	2.21	0.41
1:B:261:SER:O	1:B:262:GLN:CB	2.68	0.41
1:B:288:GLN:HA	1:B:289:PRO:HD2	1.89	0.41
1:C:317:LEU:C	1:C:317:LEU:CD2	2.93	0.41
1:A:272:LYS:HD3	1:A:272:LYS:HA	1.95	0.41
1:B:313:ALA:HB1	1:B:473:ALA:CB	2.49	0.41
1:B:370:VAL:HG22	1:B:411:ILE:HD13	2.03	0.41
1:B:462:THR:HG22	1:B:465:GLU:CB	2.51	0.41
1:B:259:SER:C	1:B:260:ARG:HG3	2.46	0.40
1:B:383:THR:C	1:B:385:LYS:N	2.76	0.40
1:C:264:LYS:HG2	1:C:268:ASP:OD2	2.21	0.40
1:A:351:VAL:HG22	1:A:373:MET:SD	2.62	0.40
1:B:400:ARG:HH11	1:B:410:GLN:HG2	1.87	0.40
1:A:310:GLN:HB2	2:A:556:HOH:O	2.20	0.40
1:C:412:ASP:O	1:C:414:THR:HG23	2.20	0.40
1:C:472:TRP:CD1	1:C:476:HIS:CE1	3.09	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

There are no protein backbone outliers to report in this entry.

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	217/229 (95%)	201 (93%)	16 (7%)	13	22
1	B	212/229 (93%)	203 (96%)	9 (4%)	26	45
1	C	132/229 (58%)	122 (92%)	10 (8%)	12	21
All	All	561/687 (82%)	526 (94%)	35 (6%)	16	29

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	225	MET
1	A	260	ARG
1	A	297	ARG
1	A	315	VAL
1	A	321	THR
1	A	351	VAL
1	A	356	CYS
1	A	359	TRP
1	A	360	THR
1	A	364	PHE
1	A	383	THR
1	A	419	THR
1	A	433	THR
1	A	453	ARG
1	A	461	VAL
1	A	479	GLU
1	B	237	THR
1	B	240	LYS
1	B	253	PHE

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Mol	Chain	Res	Type
1	B	293	ILE
1	B	338	THR
1	B	361	ASN
1	B	362	GLU
1	B	419	THR
1	B	462	THR
1	C	237	THR
1	C	272	LYS
1	C	273	ILE
1	C	277	THR
1	C	322	LYS
1	C	329	THR
1	C	415	PRO
1	C	442	GLN
1	C	478	VAL
1	C	483	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	241	GLN
1	A	254	ASN
1	A	269	ASN
1	A	287	GLN
1	A	342	ASN
1	A	349	HIS
1	A	361	ASN
1	A	367	ASN
1	A	423	ASN
1	A	437	HIS
1	A	439	GLN
1	A	476	HIS
1	B	305	ASN
1	B	310	GLN
1	B	361	ASN
1	B	363	ASN
1	B	403	GLN
1	B	438	GLN
1	B	464	GLN
1	B	482	HIS
1	C	244	GLN
1	C	258	ASN

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Mol	Chain	Res	Type
1	C	482	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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.