



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:39 AM UTC

PDB ID : 3EB8 / pdb_00003eb8
Title : VirA
Authors : Germane, K.L.; Spiller, B.W.
Deposited on : 2008-08-27
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
Xtrriage (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

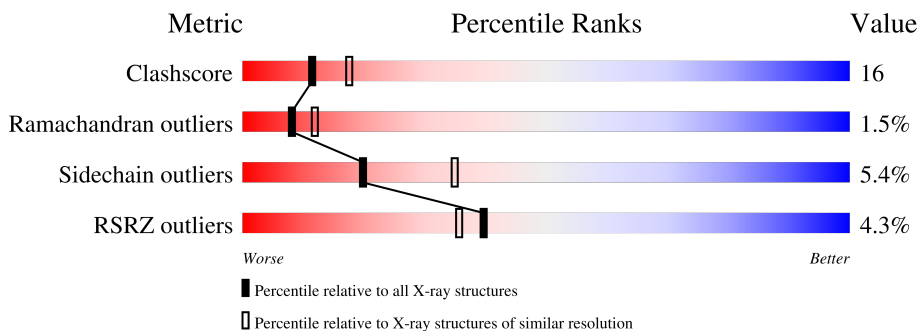
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 $\leq 5\%$. 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	358	
1	B	358	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5371 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 Cysteine protease-like virA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	334	2634	1667	443	512	12	0	0	0
1	B	336	2646	1675	445	514	12	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	43	GLY	-	expression tag	UNP Q7BU69
A	44	SER	-	expression tag	UNP Q7BU69
B	43	GLY	-	expression tag	UNP Q7BU69
B	44	SER	-	expression tag	UNP Q7BU69

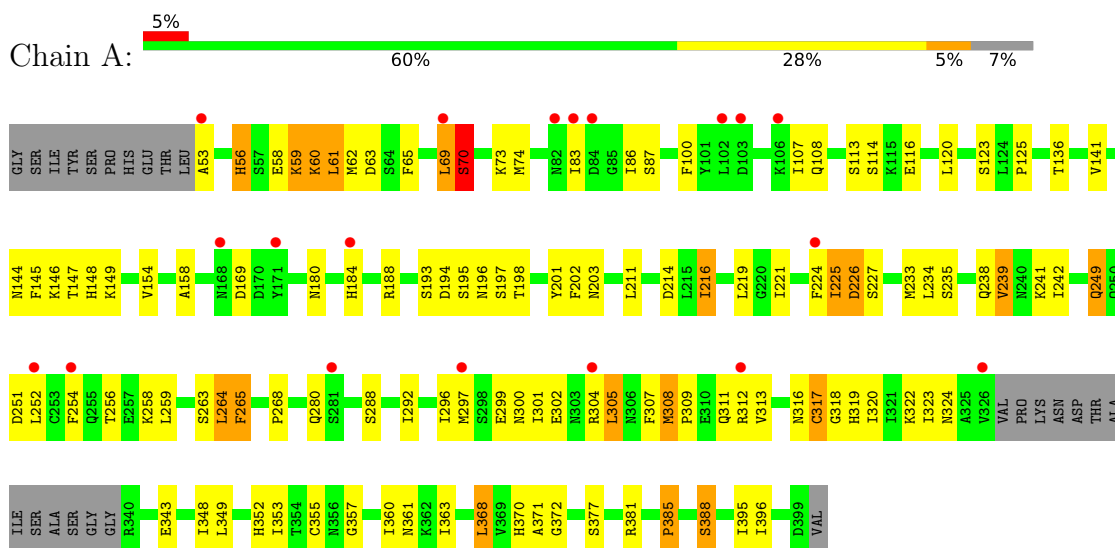
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	26	Total	O	0	0
			26	26		
2	B	65	Total	O	0	0
			65	65		

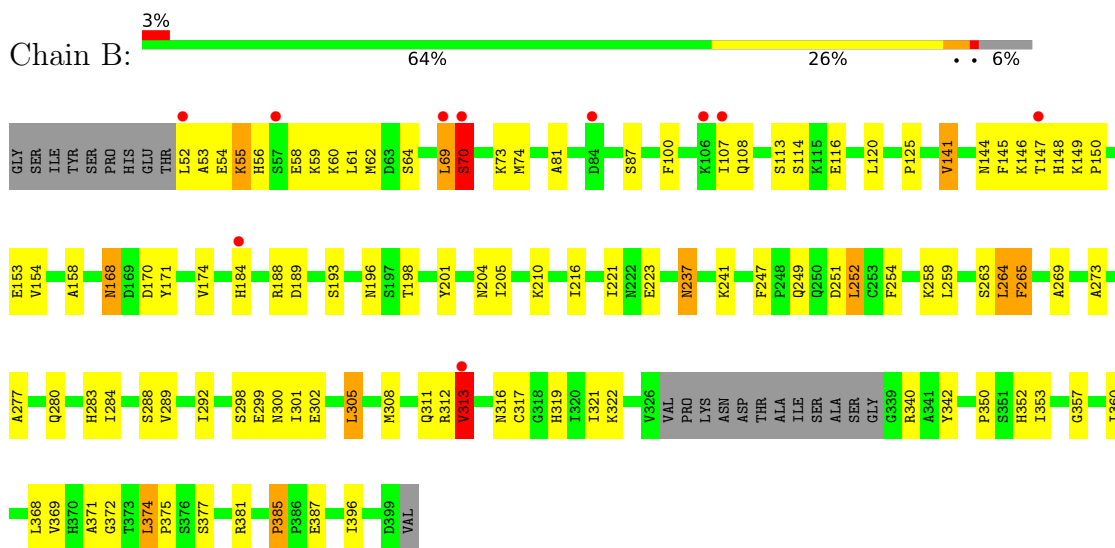
3 Residue-property plots [i](#)

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: Cysteine protease-like virA



- Molecule 1: Cysteine protease-like virA



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	91.29Å 91.29Å 198.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.99 – 2.40 39.99 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.5 (39.99-2.40) 99.5 (39.99-2.40)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.51 (at 2.39Å)	Xtrriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.217 , 0.267 0.216 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	52.7	Xtrriage
Anisotropy	0.054	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5371	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.23% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.53	0/2689	0.87	7/3645 (0.2%)
1	B	0.54	0/2701	0.90	10/3661 (0.3%)
All	All	0.54	0/5390	0.88	17/7306 (0.2%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	LEU	N-CA-C	-9.34	98.61	110.19
1	A	264	LEU	N-CA-C	-7.63	100.49	110.33
1	B	264	LEU	N-CA-C	-6.56	101.87	110.33
1	B	372	GLY	N-CA-C	6.53	121.86	114.67
1	B	374	LEU	CA-C-N	6.10	127.47	119.84
1	B	374	LEU	C-N-CA	6.10	127.47	119.84
1	B	55	LYS	N-CA-C	-6.09	106.11	112.93
1	A	385	PRO	O-C-N	5.97	123.96	121.15
1	B	69	LEU	N-CA-C	-5.74	106.41	113.41
1	B	284	ILE	N-CA-C	5.66	112.27	106.21
1	A	69	LEU	N-CA-C	-5.53	106.67	113.41
1	B	313	VAL	N-CA-C	5.39	120.56	109.34
1	A	371	ALA	N-CA-C	5.39	117.85	111.33
1	B	385	PRO	CA-C-N	5.26	126.41	119.84
1	B	385	PRO	C-N-CA	5.26	126.41	119.84
1	A	308	MET	CA-C-N	5.00	124.61	119.05
1	A	308	MET	C-N-CA	5.00	124.61	119.05

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	2634	0	2596	98	0
1	B	2646	0	2610	89	0
2	A	26	0	0	1	0
2	B	65	0	0	0	0
All	All	5371	0	5206	169	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 16.

All (169) 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:63:ASP:HA	1:A:125:PRO:HG3	1.58	0.85
1:A:300:ASN:ND2	1:A:353:ILE:H	1.76	0.83
1:B:193:SER:HA	1:B:196:ASN:HB2	1.62	0.82
1:A:300:ASN:HD22	1:A:353:ILE:H	1.26	0.80
1:A:264:LEU:O	1:A:265:PHE:HB2	1.84	0.77
1:B:300:ASN:HD22	1:B:353:ILE:H	1.33	0.77
1:B:216:ILE:HG23	1:B:221:ILE:HB	1.66	0.76
1:A:193:SER:HA	1:A:196:ASN:HB2	1.67	0.75
1:A:297:MET:HB3	1:B:305:LEU:HD21	1.67	0.74
1:A:252:LEU:O	1:A:256:THR:HG23	1.89	0.73
1:B:237:ASN:HD22	1:B:237:ASN:H	1.35	0.71
1:A:194:ASP:O	1:B:223:GLU:HG2	1.90	0.71
1:B:264:LEU:O	1:B:265:PHE:HB2	1.88	0.71
1:B:251:ASP:HB3	1:B:254:PHE:HD1	1.55	0.70
1:A:301:ILE:HG12	1:B:301:ILE:CG2	2.22	0.69
1:A:249:GLN:HB2	1:A:254:PHE:CD1	2.27	0.69
1:A:188:ARG:HH11	1:B:312:ARG:NH2	1.90	0.69
1:A:113:SER:OG	1:A:116:GLU:HG3	1.94	0.68
1:A:233:MET:HG3	1:A:268:PRO:HG3	1.74	0.68
1:A:148:HIS:CD2	1:A:312:ARG:HH12	2.13	0.67
1:B:300:ASN:ND2	1:B:353:ILE:H	1.94	0.66
1:A:196:ASN:HB3	1:A:198:THR:H	1.61	0.64
1:B:144:ASN:ND2	1:B:146:LYS:H	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:PRO:HG2	1:B:317:CYS:SG	2.38	0.63
1:A:74:MET:HE1	1:A:100:PHE:CD2	2.34	0.63
1:B:52:LEU:N	1:B:55:LYS:HZ3	1.96	0.62
1:A:300:ASN:HB2	1:A:352:HIS:CD2	2.35	0.62
1:B:113:SER:OG	1:B:116:GLU:HG3	1.99	0.62
1:B:74:MET:HE1	1:B:100:PHE:CD2	2.35	0.61
1:A:70:SER:O	1:A:73:LYS:HD3	2.01	0.61
1:A:144:ASN:ND2	1:A:146:LYS:H	2.00	0.59
1:B:269:ALA:HB2	1:B:371:ALA:O	2.02	0.59
1:A:301:ILE:HD11	1:B:305:LEU:HD23	1.86	0.58
1:A:385:PRO:HG2	1:A:388:SER:OG	2.02	0.58
1:B:201:TYR:CD1	1:B:322:LYS:HE3	2.39	0.58
1:A:320:ILE:HD13	1:A:349:LEU:HD11	1.86	0.58
1:B:70:SER:O	1:B:73:LYS:HD3	2.04	0.58
1:A:305:LEU:HD21	1:B:298:SER:HB3	1.85	0.58
1:A:61:LEU:O	1:A:62:MET:HB2	2.03	0.58
1:B:61:LEU:O	1:B:62:MET:HB2	2.04	0.58
1:B:249:GLN:H	1:B:249:GLN:CD	2.12	0.57
1:B:316:ASN:CB	1:B:350:PRO:HA	2.34	0.57
1:A:216:ILE:HG13	1:A:221:ILE:HD12	1.86	0.57
1:A:305:LEU:HD21	1:B:298:SER:CB	2.35	0.57
1:A:381:ARG:HD3	2:A:417:HOH:O	2.05	0.56
1:B:74:MET:HE1	1:B:100:PHE:CE2	2.40	0.56
1:A:203:ASN:HA	1:A:324:ASN:OD1	2.06	0.56
1:B:193:SER:CA	1:B:196:ASN:HB2	2.35	0.56
1:B:254:PHE:O	1:B:258:LYS:HG3	2.05	0.56
1:A:201:TYR:CD1	1:A:322:LYS:HE2	2.41	0.55
1:A:211:LEU:CD1	1:A:242:ILE:HG22	2.35	0.55
1:B:144:ASN:HD22	1:B:146:LYS:H	1.53	0.55
1:B:299:GLU:OE1	1:B:352:HIS:HE1	1.90	0.54
1:A:144:ASN:HD22	1:A:146:LYS:H	1.55	0.54
1:A:249:GLN:NE2	1:A:249:GLN:H	2.05	0.54
1:A:297:MET:CB	1:B:305:LEU:HD21	2.38	0.53
1:A:74:MET:HE1	1:A:100:PHE:CE2	2.44	0.53
1:A:307:PHE:CE1	1:A:355:CYS:HA	2.44	0.53
1:A:263:SER:C	1:A:264:LEU:O	2.50	0.52
1:A:225:ILE:O	1:A:226:ASP:HB3	2.09	0.52
1:A:254:PHE:O	1:A:258:LYS:HG3	2.10	0.52
1:A:195:SER:HB3	1:B:223:GLU:CD	2.34	0.52
1:B:252:LEU:C	1:B:252:LEU:HD12	2.35	0.52
1:B:147:THR:HG22	1:B:149:LYS:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:SER:O	1:A:239:VAL:HG13	2.10	0.51
1:B:148:HIS:CD2	1:B:312:ARG:HH12	2.28	0.51
1:B:145:PHE:CE2	1:B:357:GLY:HA2	2.46	0.51
1:A:154:VAL:HG12	1:A:360:ILE:HD12	1.92	0.51
1:B:154:VAL:HG12	1:B:360:ILE:HD12	1.92	0.51
1:A:300:ASN:HD22	1:A:353:ILE:N	2.02	0.50
1:B:193:SER:HA	1:B:196:ASN:CB	2.38	0.50
1:A:120:LEU:C	1:A:120:LEU:HD23	2.37	0.50
1:A:370:HIS:HD2	1:A:372:GLY:H	1.58	0.50
1:B:316:ASN:HB2	1:B:350:PRO:HA	1.92	0.50
1:A:62:MET:HA	1:A:65:PHE:HD1	1.77	0.50
1:B:62:MET:O	1:B:125:PRO:HG3	2.11	0.50
1:B:277:ALA:HB1	1:B:321:ILE:HD12	1.93	0.50
1:A:305:LEU:HD21	1:B:298:SER:OG	2.11	0.50
1:B:288:SER:O	1:B:292:ILE:HG12	2.11	0.50
1:A:147:THR:HG22	1:A:149:LYS:H	1.76	0.49
1:B:184:HIS:HB3	1:B:188:ARG:HH21	1.77	0.49
1:B:263:SER:C	1:B:264:LEU:O	2.52	0.49
1:A:61:LEU:CD2	1:A:83:ILE:HD13	2.42	0.49
1:B:120:LEU:C	1:B:120:LEU:HD23	2.38	0.49
1:B:52:LEU:O	1:B:53:ALA:HB3	2.13	0.49
1:B:158:ALA:HA	1:B:396:ILE:HG12	1.95	0.49
1:A:62:MET:HE2	1:A:123:SER:OG	2.12	0.49
1:A:145:PHE:CE2	1:A:357:GLY:HA2	2.48	0.49
1:B:300:ASN:HB2	1:B:352:HIS:CD2	2.48	0.49
1:A:312:ARG:NH1	1:B:280:GLN:HE22	2.11	0.49
1:B:62:MET:C	1:B:64:SER:N	2.68	0.49
1:A:225:ILE:O	1:A:226:ASP:CB	2.61	0.48
1:B:52:LEU:HD23	1:B:55:LYS:HD3	1.95	0.48
1:B:196:ASN:HB3	1:B:198:THR:H	1.78	0.48
1:A:62:MET:HA	1:A:65:PHE:CD1	2.49	0.48
1:A:308:MET:HB2	1:A:311:GLN:HB3	1.95	0.48
1:B:189:ASP:OD1	1:B:319:HIS:HD2	1.95	0.48
1:A:184:HIS:HB3	1:A:188:ARG:HH21	1.79	0.48
1:A:53:ALA:HA	1:A:56:HIS:CE1	2.49	0.48
1:B:340:ARG:O	1:B:371:ALA:HA	2.13	0.48
1:A:197:SER:HB2	1:A:317:CYS:O	2.13	0.48
1:B:148:HIS:O	1:B:313:VAL:HA	2.13	0.48
1:A:301:ILE:HG12	1:B:301:ILE:HG23	1.95	0.48
1:A:219:LEU:HD23	1:A:234:LEU:CD1	2.45	0.47
1:A:61:LEU:HD22	1:A:83:ILE:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:HIS:O	1:B:289:VAL:HG11	2.15	0.47
1:A:59:LYS:HB2	1:A:59:LYS:HE2	1.63	0.47
1:A:377:SER:O	1:A:381:ARG:HG2	2.15	0.47
1:A:304:ARG:HD3	1:B:301:ILE:HD11	1.98	0.46
1:B:374:LEU:HA	1:B:375:PRO:HD3	1.78	0.46
1:A:188:ARG:HH11	1:B:312:ARG:CZ	2.28	0.46
1:A:296:ILE:HG21	1:A:361:ASN:ND2	2.30	0.46
1:B:147:THR:HG22	1:B:148:HIS:N	2.30	0.46
1:A:60:LYS:C	1:A:61:LEU:O	2.53	0.46
1:A:288:SER:O	1:A:292:ILE:HG12	2.15	0.46
1:B:54:GLU:C	1:B:56:HIS:H	2.24	0.46
1:A:249:GLN:HB2	1:A:254:PHE:CG	2.51	0.46
1:B:308:MET:HB2	1:B:311:GLN:HB3	1.96	0.46
1:A:202:PHE:HA	1:A:323:ILE:O	2.16	0.45
1:B:52:LEU:CD2	1:B:55:LYS:HD3	2.47	0.45
1:B:171:TYR:CD1	1:B:387:GLU:HB3	2.51	0.45
1:B:174:VAL:CG2	1:B:385:PRO:HB3	2.46	0.45
1:A:69:LEU:O	1:A:70:SER:C	2.61	0.44
1:A:147:THR:HG22	1:A:148:HIS:N	2.32	0.44
1:A:305:LEU:O	1:A:309:PRO:HG3	2.17	0.44
1:A:316:ASN:CG	1:A:318:GLY:H	2.24	0.44
1:A:348:ILE:HG22	1:A:363:ILE:HB	1.98	0.44
1:B:53:ALA:O	1:B:56:HIS:ND1	2.46	0.44
1:A:301:ILE:HD11	1:B:305:LEU:HB2	2.00	0.43
1:B:193:SER:O	1:B:196:ASN:HB2	2.18	0.43
1:B:247:PHE:HB2	1:B:258:LYS:HG2	1.99	0.43
1:A:58:GLU:O	1:A:62:MET:HG2	2.18	0.43
1:A:148:HIS:CG	1:A:312:ARG:HH12	2.36	0.43
1:A:251:ASP:HB2	1:A:254:PHE:HD1	1.84	0.43
1:A:280:GLN:NE2	1:B:312:ARG:HB2	2.33	0.43
1:B:168:ASN:O	1:B:170:ASP:N	2.51	0.43
1:A:249:GLN:HE21	1:A:249:GLN:N	2.16	0.43
1:B:54:GLU:O	1:B:58:GLU:HG3	2.19	0.42
1:A:158:ALA:HA	1:A:396:ILE:HG12	2.00	0.42
1:B:193:SER:HA	1:B:196:ASN:ND2	2.34	0.42
1:B:377:SER:O	1:B:381:ARG:HG2	2.19	0.42
1:A:198:THR:HA	1:A:319:HIS:O	2.19	0.42
1:A:184:HIS:HB3	1:A:188:ARG:HE	1.84	0.42
1:B:69:LEU:O	1:B:70:SER:C	2.62	0.42
1:B:210:LYS:HA	1:B:210:LYS:HD2	1.66	0.42
1:A:214:ASP:CB	1:A:242:ILE:HG23	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:GLU:OE1	1:A:352:HIS:HE1	2.03	0.42
1:B:396:ILE:HD12	1:B:396:ILE:N	2.34	0.42
1:B:237:ASN:H	1:B:237:ASN:ND2	2.08	0.42
1:B:273:ALA:HA	1:B:369:VAL:HG21	2.02	0.41
1:A:301:ILE:HG12	1:B:301:ILE:HG21	1.98	0.41
1:A:62:MET:O	1:A:125:PRO:HG3	2.20	0.41
1:A:180:ASN:O	1:A:227:SER:HB2	2.20	0.41
1:B:81:ALA:O	1:B:87:SER:HA	2.19	0.41
1:A:249:GLN:NE2	1:A:249:GLN:N	2.68	0.41
1:B:150:PRO:HG2	1:B:317:CYS:HG	1.85	0.41
1:A:238:GLN:O	1:A:241:LYS:HB3	2.20	0.41
1:A:86:ILE:HG22	1:A:87:SER:N	2.35	0.41
1:A:136:THR:HA	1:A:395:ILE:O	2.20	0.41
1:A:343:GLU:HG2	1:A:368:LEU:CD1	2.50	0.41
1:B:141:VAL:HG13	1:B:153:GLU:CD	2.46	0.41
1:B:184:HIS:HB3	1:B:188:ARG:HE	1.86	0.41
1:A:61:LEU:O	1:A:62:MET:CB	2.66	0.41
1:A:188:ARG:NH1	1:B:312:ARG:CZ	2.85	0.40
1:B:342:TYR:O	1:B:368:LEU:HD12	2.20	0.40
1:A:148:HIS:CG	1:A:312:ARG:NH1	2.89	0.40
1:B:193:SER:C	1:B:196:ASN:HB2	2.47	0.40
1:A:62:MET:CA	1:A:65:PHE:HD1	2.34	0.40
1:A:86:ILE:CG2	1:A:87:SER:N	2.84	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	330/358 (92%)	306 (93%)	19 (6%)	5 (2%)	8 12
1	B	332/358 (93%)	306 (92%)	21 (6%)	5 (2%)	8 12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	662/716 (92%)	612 (92%)	40 (6%)	10 (2%)	8	12

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	70	SER
1	A	70	SER
1	A	313	VAL
1	B	313	VAL
1	A	226	ASP
1	A	265	PHE
1	B	168	ASN
1	B	265	PHE
1	A	107	ILE
1	B	107	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	305/324 (94%)	286 (94%)	19 (6%)	16	29
1	B	306/324 (94%)	292 (95%)	14 (5%)	24	41
All	All	611/648 (94%)	578 (95%)	33 (5%)	20	35

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	HIS
1	A	59	LYS
1	A	60	LYS
1	A	70	SER
1	A	108	GLN
1	A	114	SER
1	A	141	VAL
1	A	169	ASP

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Mol	Chain	Res	Type
1	A	216	ILE
1	A	224	PHE
1	A	225	ILE
1	A	239	VAL
1	A	249	GLN
1	A	259	LEU
1	A	302	GLU
1	A	305	LEU
1	A	317	CYS
1	A	368	LEU
1	A	388	SER
1	B	59	LYS
1	B	60	LYS
1	B	70	SER
1	B	108	GLN
1	B	114	SER
1	B	141	VAL
1	B	204	ASN
1	B	205	ILE
1	B	237	ASN
1	B	241	LYS
1	B	252	LEU
1	B	259	LEU
1	B	302	GLU
1	B	305	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	GLN
1	A	118	ASN
1	A	144	ASN
1	A	148	HIS
1	A	249	GLN
1	A	280	GLN
1	A	291	HIS
1	A	300	ASN
1	A	311	GLN
1	A	315	ASN
1	A	319	HIS
1	A	352	HIS
1	A	361	ASN

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Mol	Chain	Res	Type
1	A	370	HIS
1	A	390	GLN
1	B	111	GLN
1	B	118	ASN
1	B	144	ASN
1	B	148	HIS
1	B	237	ASN
1	B	255	GLN
1	B	280	GLN
1	B	291	HIS
1	B	300	ASN
1	B	315	ASN
1	B	319	HIS
1	B	352	HIS
1	B	361	ASN
1	B	390	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 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

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	334/358 (93%)	0.44	19 (5%) 29 25	45, 61, 97, 133	0
1	B	336/358 (93%)	0.23	10 (2%) 52 48	38, 53, 98, 141	0
All	All	670/716 (93%)	0.34	29 (4%) 40 36	38, 57, 97, 141	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	53	ALA	4.6
1	A	103	ASP	4.5
1	A	84	ASP	4.5
1	A	168	ASN	4.1
1	B	52	LEU	3.6
1	B	107	ILE	3.4
1	B	147	THR	3.2
1	B	313	VAL	3.0
1	A	106	LYS	2.8
1	B	69	LEU	2.8
1	A	82	ASN	2.6
1	B	184	HIS	2.5
1	B	106	LYS	2.4
1	A	297	MET	2.4
1	B	57	SER	2.4
1	A	312	ARG	2.4
1	A	304	ARG	2.4
1	B	84	ASP	2.3
1	A	254	PHE	2.3
1	A	83	ILE	2.3
1	A	252	LEU	2.3
1	A	102	LEU	2.3
1	A	326	VAL	2.3
1	A	281	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	69	LEU	2.2
1	B	70	SER	2.1
1	A	171	TYR	2.1
1	A	184	HIS	2.1
1	A	224	PHE	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.