



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:29 PM UTC

PDB ID : 4IKA / pdb_00004ika
Title : Crystal structure of EV71 3Dpol-VPg
Authors : Chen, C.; Wang, Y.X.; Lou, Z.Y.
Deposited on : 2012-12-25
Resolution : 2.70 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)	:	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

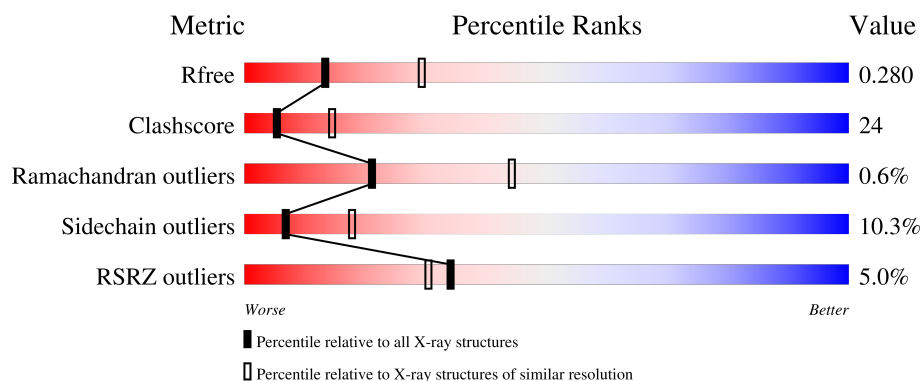
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	462	3% 56% 37% 6%
2	D	22	45% 9% 59% 23% 9%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4170 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 3Dpol.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	462	Total	C	N	O	S	0	0	0
			3700	2368	619	695	18			

- Molecule 2 is a protein called VPg.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	20	Total	C	N	O	0	0	0
			144	92	27	25			

- Molecule 3 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Ni	0	0
			2	2		

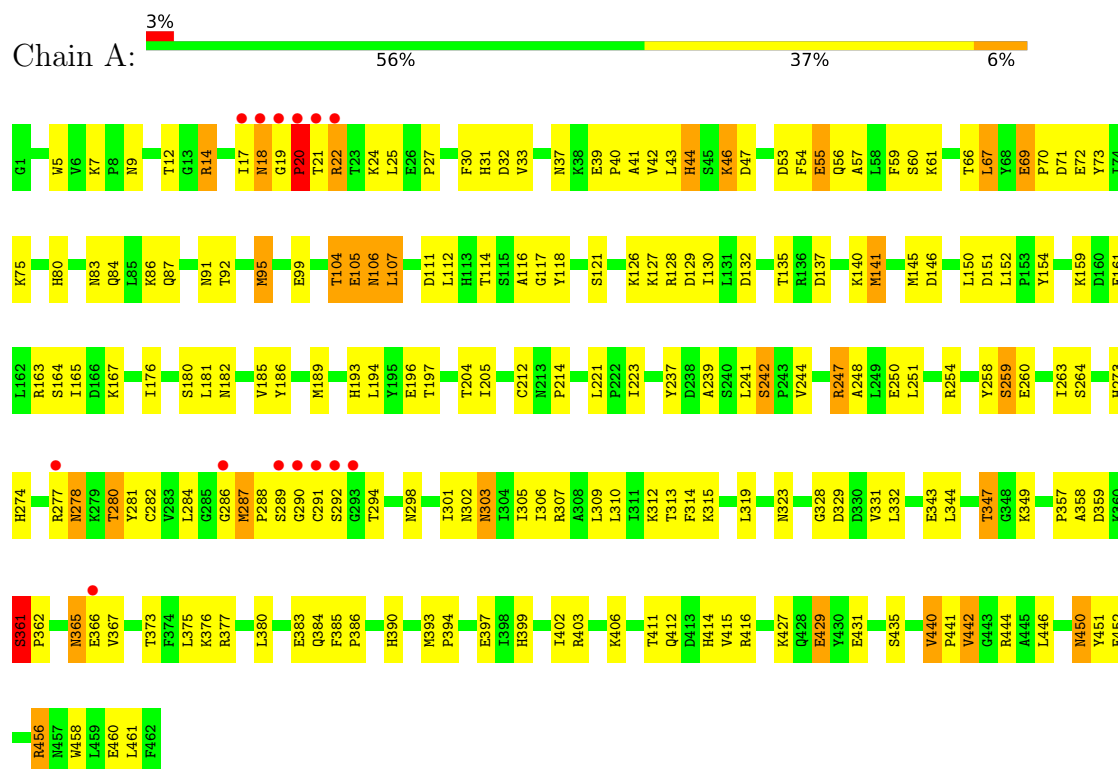
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	310	Total	O	0	0
			310	310		
4	D	14	Total	O	0	0
			14	14		

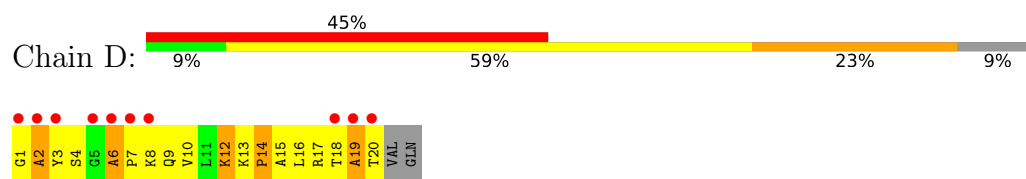
3 Residue-property plots [i](#)

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: 3Dpol



• Molecule 2: VPg



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	103.60Å 103.60Å 132.17Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.23 – 2.70 48.23 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.23-2.70) 90.1 (48.23-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.35 (at 2.42Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.218 , 0.278 0.225 , 0.280	Depositor DCC
R_{free} test set	1268 reflections (3.99%)	wwPDB-VP
Wilson B-factor (Å ²)	47.7	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 53.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.034 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4170	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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 ⓘ

5.1 Standard geometry ⓘ

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

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	0.55	2/3795 (0.1%)	1.02	21/5144 (0.4%)
2	D	0.77	2/146 (1.4%)	1.74	6/196 (3.1%)
All	All	0.56	4/3941 (0.1%)	1.05	27/5340 (0.5%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	362	PRO	N-CD	6.51	1.56	1.47
2	D	13	LYS	C-N	5.75	1.41	1.33
2	D	14	PRO	N-CD	5.15	1.54	1.47
1	A	20	PRO	N-CD	5.05	1.54	1.47

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	18	ASN	CB-CA-C	-24.36	76.02	112.07
2	D	4	SER	N-CA-C	12.54	128.79	110.10
2	D	19	ALA	N-CA-C	-9.34	93.07	108.67
2	D	4	SER	N-CA-CB	-8.82	96.20	109.69
1	A	289	SER	N-CA-C	8.48	124.23	113.55
2	D	20	THR	N-CA-CB	7.95	125.02	111.50
1	A	107	LEU	N-CA-CB	7.88	121.87	110.37
1	A	66	THR	N-CA-C	7.32	122.27	113.12
1	A	289	SER	CB-CA-C	-6.97	98.53	109.34
2	D	13	LYS	CA-C-N	-6.61	112.96	119.76
2	D	13	LYS	C-N-CA	-6.61	112.96	119.76
1	A	106	ASN	CB-CA-C	-6.60	97.29	110.42
1	A	278	ASN	N-CA-C	6.49	124.63	110.80
1	A	361	SER	CB-CA-C	-6.41	99.39	109.52
1	A	66	THR	CB-CA-C	-5.92	99.79	109.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	152	LEU	CA-C-N	5.45	125.21	119.76
1	A	152	LEU	C-N-CA	5.45	125.21	119.76
1	A	69	GLU	CA-C-N	5.35	125.27	119.76
1	A	69	GLU	C-N-CA	5.35	125.27	119.76
1	A	361	SER	N-CA-C	5.34	116.43	109.64
1	A	19	GLY	CA-C-N	-5.18	113.37	119.84
1	A	19	GLY	C-N-CA	-5.18	113.37	119.84
1	A	116	ALA	N-CA-C	-5.17	103.86	110.53
1	A	385	PHE	CA-C-N	5.13	126.25	119.84
1	A	385	PHE	C-N-CA	5.13	126.25	119.84
1	A	104	THR	N-CA-C	-5.11	101.69	108.74
1	A	118	TYR	N-CA-C	-5.09	103.61	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	3700	0	3634	175	1
2	D	144	0	161	17	0
3	A	2	0	0	0	0
4	A	310	0	0	15	1
4	D	14	0	0	1	0
All	All	4170	0	3795	184	1

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 24.

All (184) 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:117:GLY:HA3	1:A:180:SER:HA	1.20	1.17
2:D:12:LYS:HE2	2:D:12:LYS:HA	1.16	1.13
1:A:313:THR:OG1	1:A:347:THR:HG21	1.45	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ASN:O	1:A:18:ASN:CG	1.84	1.04
1:A:185:VAL:HG12	1:A:189:MET:HE2	1.43	0.98
1:A:46:LYS:H	1:A:46:LYS:HD2	1.31	0.93
1:A:366:GLU:O	4:A:801:HOH:O	1.87	0.93
1:A:20:PRO:O	1:A:21:THR:OG1	1.87	0.92
1:A:359:ASP:OD1	1:A:373:THR:HB	1.79	0.83
2:D:12:LYS:HA	2:D:12:LYS:CE	2.05	0.80
1:A:186:TYR:HA	1:A:189:MET:HE3	1.67	0.77
1:A:397:GLU:OE1	4:A:644:HOH:O	2.01	0.77
1:A:376:LYS:HD2	1:A:393:MET:HE1	1.70	0.73
2:D:6:ALA:HB3	2:D:7:PRO:HD3	1.68	0.73
1:A:105:GLU:O	1:A:106:ASN:HB2	1.88	0.73
1:A:137:ASP:OD2	4:A:693:HOH:O	2.07	0.73
1:A:273:HIS:CD2	4:A:602:HOH:O	2.41	0.72
2:D:12:LYS:HE2	2:D:12:LYS:CA	2.08	0.72
1:A:140:LYS:HD3	4:A:627:HOH:O	1.88	0.72
1:A:315:LYS:HG3	2:D:17:ARG:NH1	2.05	0.71
1:A:291:CYS:O	1:A:294:THR:OG1	2.07	0.71
1:A:290:GLY:HA2	4:A:802:HOH:O	1.90	0.71
1:A:132:ASP:OD2	1:A:135:THR:HG23	1.92	0.70
1:A:20:PRO:HD2	1:A:21:THR:H	1.56	0.70
1:A:365:ASN:HB3	4:A:801:HOH:O	1.91	0.70
1:A:114:THR:O	1:A:127:LYS:HE3	1.91	0.69
1:A:46:LYS:HD2	1:A:46:LYS:N	2.06	0.68
1:A:164:SER:H	1:A:167:LYS:CE	2.07	0.67
1:A:18:ASN:C	1:A:18:ASN:OD1	2.32	0.66
1:A:456:ARG:HG2	4:A:780:HOH:O	1.94	0.66
1:A:377:ARG:HG3	1:A:377:ARG:HH11	1.61	0.66
1:A:313:THR:HG1	1:A:347:THR:HG21	1.60	0.66
1:A:247:ARG:NH1	1:A:250:GLU:OE1	2.29	0.65
1:A:429:GLU:H	1:A:429:GLU:CD	2.03	0.65
1:A:291:CYS:HB3	1:A:294:THR:OG1	1.96	0.65
1:A:427:LYS:O	1:A:431:GLU:HG2	1.96	0.65
1:A:247:ARG:HH11	1:A:247:ARG:HA	1.61	0.64
1:A:313:THR:OG1	1:A:347:THR:CG2	2.36	0.64
1:A:71:ASP:O	1:A:75:LYS:HG3	1.98	0.63
1:A:309:LEU:HB3	1:A:344:LEU:HD22	1.80	0.63
1:A:440:VAL:CG1	1:A:442:VAL:HG23	2.29	0.62
1:A:431:GLU:HG3	4:A:607:HOH:O	1.99	0.62
1:A:273:HIS:HD2	4:A:602:HOH:O	1.77	0.62
1:A:312:LYS:O	2:D:17:ARG:HG3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:GLU:HG3	2:D:16:LEU:HD11	1.83	0.61
1:A:254:ARG:NH1	1:A:260:GLU:OE1	2.28	0.61
1:A:298:ASN:HB3	1:A:328:GLY:HA2	1.82	0.61
1:A:80:HIS:ND1	1:A:319:LEU:HB3	2.16	0.60
1:A:21:THR:OG1	1:A:44:HIS:HD2	1.83	0.60
1:A:414:HIS:HD2	4:A:721:HOH:O	1.84	0.60
1:A:126:LYS:O	1:A:129:ASP:HB2	2.01	0.60
1:A:164:SER:HB3	1:A:167:LYS:HE2	1.83	0.60
1:A:27:PRO:HB3	1:A:31:HIS:CG	2.37	0.59
1:A:106:ASN:O	1:A:196:GLU:HA	2.02	0.59
1:A:39:GLU:HB2	1:A:40:PRO:HD2	1.85	0.58
1:A:53:ASP:O	1:A:56:GLN:HB3	2.04	0.58
1:A:393:MET:HE3	1:A:394:PRO:HD2	1.85	0.58
1:A:130:ILE:HG21	1:A:141:MET:HE2	1.85	0.58
1:A:20:PRO:CD	1:A:21:THR:H	2.17	0.58
1:A:343:GLU:HG3	2:D:16:LEU:CD1	2.33	0.58
2:D:9:GLN:HG2	2:D:10:VAL:N	2.18	0.58
1:A:259:SER:O	1:A:263:ILE:HG13	2.03	0.57
1:A:83:ASN:HA	1:A:86:LYS:HD2	1.86	0.57
1:A:105:GLU:O	1:A:106:ASN:CB	2.52	0.57
1:A:80:HIS:HD1	1:A:319:LEU:HB3	1.70	0.57
1:A:406:LYS:HD3	4:A:614:HOH:O	2.05	0.57
1:A:20:PRO:C	1:A:21:THR:HG1	1.98	0.57
1:A:71:ASP:OD1	1:A:73:TYR:N	2.38	0.57
1:A:242:SER:HB3	1:A:244:VAL:HG12	1.85	0.57
1:A:357:PRO:HB2	1:A:361:SER:O	2.05	0.57
1:A:343:GLU:O	1:A:347:THR:HG22	2.04	0.56
1:A:46:LYS:H	1:A:46:LYS:CD	2.11	0.56
1:A:429:GLU:CD	1:A:429:GLU:N	2.65	0.55
1:A:99:GLU:HG2	1:A:104:THR:HG22	1.87	0.55
1:A:315:LYS:HG3	2:D:17:ARG:HH11	1.68	0.55
1:A:9:ASN:OD1	1:A:280:THR:HG22	2.07	0.54
1:A:164:SER:CB	1:A:167:LYS:HE2	2.38	0.54
1:A:105:GLU:O	1:A:105:GLU:HG3	2.07	0.54
1:A:95:MET:HE1	1:A:107:LEU:HD23	1.90	0.54
1:A:22:ARG:HH11	1:A:22:ARG:HG3	1.73	0.53
1:A:91:ASN:HB3	1:A:193:HIS:HB3	1.88	0.53
2:D:10:VAL:HG22	4:D:110:HOH:O	2.08	0.53
1:A:164:SER:H	1:A:167:LYS:HE3	1.74	0.53
1:A:44:HIS:HB2	1:A:46:LYS:HE3	1.91	0.53
1:A:292:SER:C	1:A:294:THR:H	2.17	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:GLN:NE2	1:A:307:ARG:NH2	2.56	0.53
1:A:41:ALA:HB2	1:A:163:ARG:HG2	1.91	0.52
1:A:159:LYS:HD3	1:A:161:GLU:CD	2.34	0.52
1:A:274:HIS:HB2	1:A:281:TYR:CZ	2.44	0.52
1:A:301:ILE:O	1:A:305:ILE:HG13	2.09	0.52
1:A:456:ARG:O	1:A:460:GLU:HG3	2.10	0.52
1:A:60:SER:OG	4:A:687:HOH:O	2.19	0.51
1:A:359:ASP:HB3	4:A:724:HOH:O	2.10	0.51
1:A:429:GLU:N	1:A:429:GLU:OE2	2.44	0.50
1:A:302:ASN:O	1:A:306:ILE:HG12	2.12	0.50
1:A:83:ASN:OD1	1:A:86:LYS:HE3	2.12	0.50
1:A:375:LEU:O	1:A:377:ARG:NH1	2.45	0.50
1:A:9:ASN:ND2	1:A:278:ASN:HA	2.27	0.49
2:D:1:GLY:O	2:D:2:ALA:HB2	2.11	0.49
1:A:241:LEU:HB2	1:A:286:GLY:HA2	1.93	0.49
1:A:314:PHE:CD2	2:D:14:PRO:HB2	2.47	0.49
1:A:12:THR:OG1	1:A:280:THR:HG21	2.13	0.48
1:A:5:TRP:CE3	1:A:7:LYS:HG3	2.49	0.48
1:A:287:MET:HE2	1:A:287:MET:HB2	1.77	0.48
1:A:117:GLY:CA	1:A:180:SER:HA	2.14	0.48
1:A:73:TYR:HE1	2:D:17:ARG:HH21	1.60	0.48
1:A:39:GLU:HB2	1:A:40:PRO:CD	2.44	0.48
1:A:375:LEU:O	1:A:376:LYS:HB2	2.14	0.48
1:A:80:HIS:CE1	1:A:319:LEU:HB3	2.48	0.48
1:A:193:HIS:HD2	1:A:196:GLU:OE1	1.96	0.48
1:A:390:HIS:CE1	1:A:458:TRP:CZ3	3.02	0.47
1:A:194:LEU:C	1:A:194:LEU:HD23	2.39	0.47
1:A:194:LEU:HB2	1:A:258:TYR:OH	2.14	0.47
1:A:54:PHE:O	1:A:57:ALA:N	2.48	0.47
1:A:159:LYS:HG3	1:A:176:ILE:HD11	1.96	0.47
1:A:411:THR:O	1:A:415:VAL:HG23	2.14	0.47
1:A:27:PRO:HB3	1:A:31:HIS:CD2	2.50	0.47
1:A:30:PHE:HA	1:A:33:VAL:HG23	1.97	0.47
1:A:25:LEU:HD21	1:A:406:LYS:HE2	1.97	0.46
1:A:292:SER:C	1:A:294:THR:N	2.73	0.46
1:A:150:LEU:HD23	1:A:182:ASN:HB3	1.96	0.46
1:A:99:GLU:HG2	1:A:104:THR:CG2	2.46	0.46
1:A:42:VAL:HG13	1:A:47:ASP:CB	2.46	0.45
1:A:384:GLN:C	1:A:386:PRO:HD3	2.41	0.45
1:A:80:HIS:HE1	1:A:319:LEU:O	1.98	0.45
1:A:24:LYS:HB2	1:A:406:LYS:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ASN:O	1:A:18:ASN:OD1	2.23	0.45
1:A:20:PRO:CD	1:A:21:THR:N	2.80	0.45
1:A:30:PHE:HA	1:A:33:VAL:CG2	2.47	0.45
1:A:254:ARG:HD3	1:A:260:GLU:OE1	2.17	0.45
1:A:61:LYS:HD2	1:A:239:ALA:HB2	1.99	0.45
1:A:383:GLU:HA	4:A:617:HOH:O	2.17	0.44
1:A:456:ARG:HB2	1:A:456:ARG:NH1	2.32	0.44
1:A:55:GLU:O	1:A:59:PHE:HD2	2.01	0.44
1:A:154:TYR:O	1:A:274:HIS:HA	2.18	0.44
1:A:84:GLN:NE2	1:A:307:ARG:HH21	2.16	0.44
1:A:44:HIS:HB2	1:A:46:LYS:CE	2.48	0.43
1:A:431:GLU:HA	1:A:431:GLU:OE2	2.18	0.43
1:A:20:PRO:O	1:A:21:THR:CB	2.64	0.43
1:A:25:LEU:CD2	1:A:406:LYS:HE2	2.48	0.43
1:A:17:ILE:HD11	1:A:121:SER:OG	2.19	0.43
1:A:358:ALA:O	1:A:361:SER:HB2	2.19	0.43
1:A:412:GLN:OE1	1:A:446:LEU:HD22	2.18	0.43
1:A:84:GLN:HE22	1:A:307:ARG:NH2	2.17	0.43
2:D:18:THR:O	2:D:19:ALA:C	2.58	0.43
1:A:451:TYR:CD1	1:A:451:TYR:C	2.97	0.43
1:A:377:ARG:HG3	1:A:377:ARG:NH1	2.30	0.42
1:A:46:LYS:O	1:A:47:ASP:C	2.61	0.42
1:A:163:ARG:HA	1:A:163:ARG:HD2	1.92	0.42
1:A:273:HIS:CE1	1:A:282:CYS:HB2	2.54	0.42
1:A:441:PRO:HA	1:A:444:ARG:NH1	2.33	0.42
1:A:67:LEU:HD13	1:A:67:LEU:HA	1.76	0.42
1:A:456:ARG:HB2	1:A:456:ARG:HH11	1.84	0.42
1:A:112:LEU:HA	1:A:127:LYS:HD2	2.00	0.42
1:A:399:HIS:O	1:A:402:ILE:HG22	2.18	0.42
2:D:7:PRO:HA	2:D:8:LYS:HA	1.70	0.42
1:A:349:LYS:HE3	1:A:349:LYS:HB2	1.85	0.42
1:A:331:VAL:CG1	1:A:332:LEU:N	2.82	0.41
1:A:287:MET:HA	1:A:288:PRO:HD3	1.94	0.41
1:A:291:CYS:O	1:A:294:THR:CB	2.67	0.41
1:A:332:LEU:HD23	1:A:332:LEU:HA	1.95	0.41
1:A:450:ASN:ND2	1:A:452:GLU:OE2	2.52	0.41
1:A:141:MET:HE3	1:A:181:LEU:CD2	2.50	0.41
1:A:140:LYS:HE3	1:A:140:LYS:HB2	1.76	0.41
1:A:212:CYS:O	1:A:214:PRO:HD3	2.20	0.41
1:A:221:LEU:HA	1:A:221:LEU:HD23	1.76	0.41
1:A:237:TYR:CG	1:A:329:ASP:HB3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:GLU:OE1	1:A:277:ARG:NH2	2.53	0.41
1:A:223:ILE:HD12	1:A:223:ILE:N	2.36	0.41
1:A:9:ASN:HB3	1:A:14:ARG:O	2.21	0.41
1:A:14:ARG:HB2	1:A:280:THR:HG21	2.03	0.41
1:A:71:ASP:OD1	1:A:71:ASP:C	2.64	0.41
1:A:315:LYS:N	2:D:15:ALA:O	2.53	0.41
1:A:380:LEU:O	1:A:390:HIS:HB2	2.20	0.41
1:A:399:HIS:O	1:A:403:ARG:HG3	2.21	0.41
1:A:359:ASP:C	1:A:361:SER:N	2.79	0.40
1:A:69:GLU:HA	1:A:70:PRO:HD3	1.81	0.40
1:A:303:ASN:O	1:A:307:ARG:HD2	2.21	0.40
1:A:205:ILE:HD12	1:A:205:ILE:N	2.37	0.40
1:A:461:LEU:HD23	1:A:461:LEU:HA	1.86	0.40
1:A:111:ASP:OD2	1:A:114:THR:HG23	2.22	0.40
1:A:248:ALA:HA	1:A:251:LEU:HD12	2.03	0.40
1:A:307:ARG:O	1:A:310:LEU:N	2.54	0.40
1:A:357:PRO:CB	1:A:361:SER:O	2.68	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:ASP:N	4:A:621:HOH:O[3_565]	2.06	0.14

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	460/462 (100%)	436 (95%)	23 (5%)	1 (0%)	43	68
2	D	18/22 (82%)	12 (67%)	4 (22%)	2 (11%)	0	0
All	All	478/484 (99%)	448 (94%)	27 (6%)	3 (1%)	21	44

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	2	ALA
2	D	6	ALA
1	A	20	PRO

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	405/406 (100%)	364 (90%)	41 (10%)	7	18
2	D	14/16 (88%)	12 (86%)	2 (14%)	3	8
All	All	419/422 (99%)	376 (90%)	43 (10%)	7	18

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	22	ARG
1	A	37	ASN
1	A	43	LEU
1	A	44	HIS
1	A	46	LYS
1	A	55	GLU
1	A	67	LEU
1	A	72	GLU
1	A	87	GLN
1	A	92	THR
1	A	95	MET
1	A	105	GLU
1	A	128	ARG
1	A	141	MET
1	A	145	MET
1	A	146	ASP
1	A	151	ASP
1	A	165	ILE
1	A	197	THR

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Mol	Chain	Res	Type
1	A	204	THR
1	A	242	SER
1	A	247	ARG
1	A	259	SER
1	A	264	SER
1	A	280	THR
1	A	284	LEU
1	A	287	MET
1	A	303	ASN
1	A	323	ASN
1	A	347	THR
1	A	361	SER
1	A	365	ASN
1	A	367	VAL
1	A	416	ARG
1	A	429	GLU
1	A	435	SER
1	A	440	VAL
1	A	442	VAL
1	A	450	ASN
1	A	456	ARG
2	D	3	TYR
2	D	12	LYS

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	44	HIS
1	A	84	GLN
1	A	273	HIS
1	A	453	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	462/462 (100%)	-0.01	14 (3%)	52	49	26, 53, 75, 104	0
2	D	20/22 (90%)	2.28	10 (50%)	0	0	30, 107, 156, 157	0
All	All	482/484 (99%)	0.08	24 (4%)	34	30	26, 53, 83, 157	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	291	CYS	6.7
1	A	20	PRO	5.6
2	D	1	GLY	5.4
1	A	21	THR	5.1
2	D	7	PRO	4.9
1	A	290	GLY	4.9
2	D	2	ALA	4.5
1	A	19	GLY	4.5
1	A	292	SER	4.2
2	D	3	TYR	4.2
1	A	18	ASN	4.0
2	D	6	ALA	3.1
1	A	277	ARG	3.1
1	A	293	GLY	3.0
2	D	8	LYS	2.9
1	A	22	ARG	2.8
2	D	5	GLY	2.4
1	A	289	SER	2.4
1	A	286	GLY	2.3
2	D	19	ALA	2.2
2	D	20	THR	2.2
1	A	366	GLU	2.0
2	D	18	THR	2.0
1	A	17	ILE	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
3	NI	A	501	1/1	0.97	0.14	89,89,89,89	0
3	NI	A	502	1/1	0.98	0.13	67,67,67,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.