



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:29 AM UTC

PDB ID : 1IMH / pdb_00001imh
Title : TonEBP/DNA COMPLEX
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Deposited on : 2001-05-10
Resolution : 2.86 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

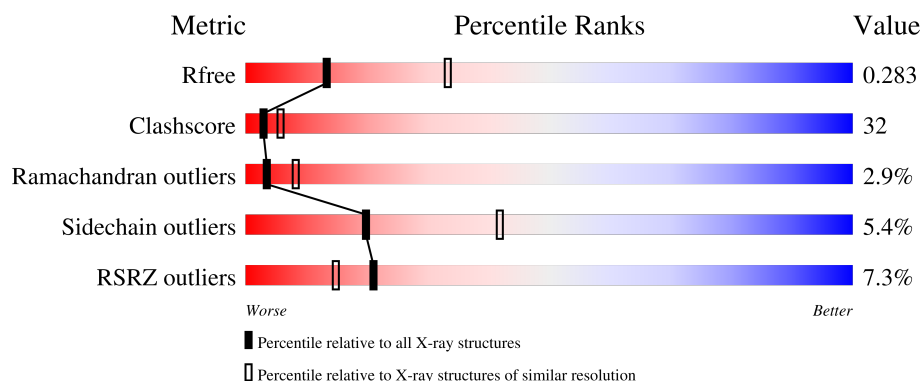
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.86 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	15	7% 7% 93%
2	B	15	20% 80%
3	C	281	7% 51% 43% 6%
3	D	281	8% 50% 45% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4977 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 DNA chain called 5'-D(*TP*TP*GP*CP*TP*GP*GP*AP*AP*AP*AP*AP*TP*AP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	15	Total	C	N	O	P	0	0	0
			310	149	61	86	14			

- Molecule 2 is a DNA chain called 5'-D(*AP*AP*CP*TP*AP*TP*TP*TP*TP*TP*CP*CP*AP*GP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	15	Total	C	N	O	P	0	0	0
			299	146	49	90	14			

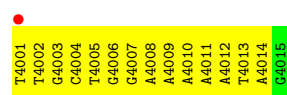
- Molecule 3 is a protein called NUCLEAR FACTOR OF ACTIVATED T CELLS 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	281	Total	C	N	O	S	0	0	0
			2184	1371	389	414	10			
3	D	281	Total	C	N	O	S	0	0	0
			2184	1371	389	414	10			

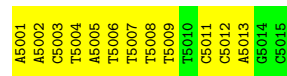
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

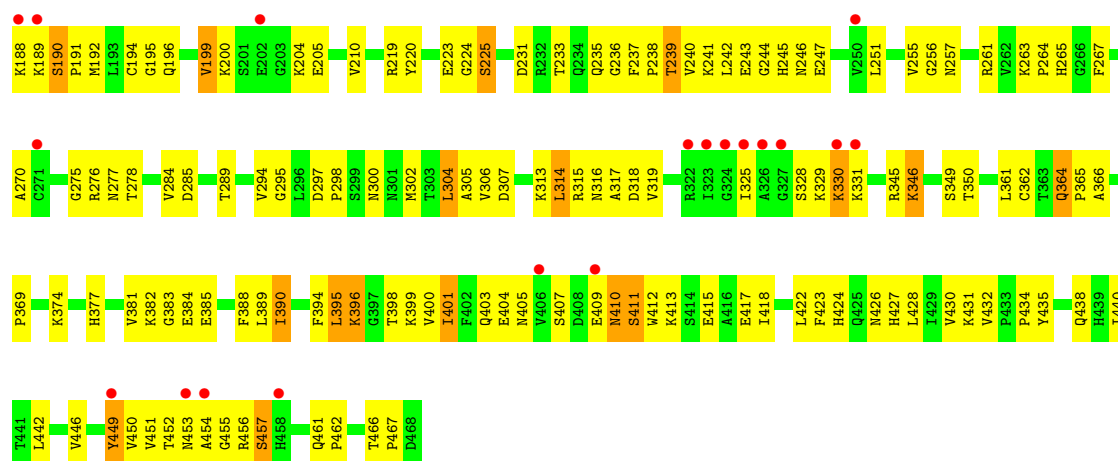
- Molecule 1: 5'-D(*TP*TP*GP*CP*TP*GP*GP*AP*AP*AP*AP*TP*AP*G)-3'



- Molecule 2: 5'-D(*AP*AP*CP*TP*AP*TP*TP*TP*TP*TP*CP*CP*AP*GP*C)-3'

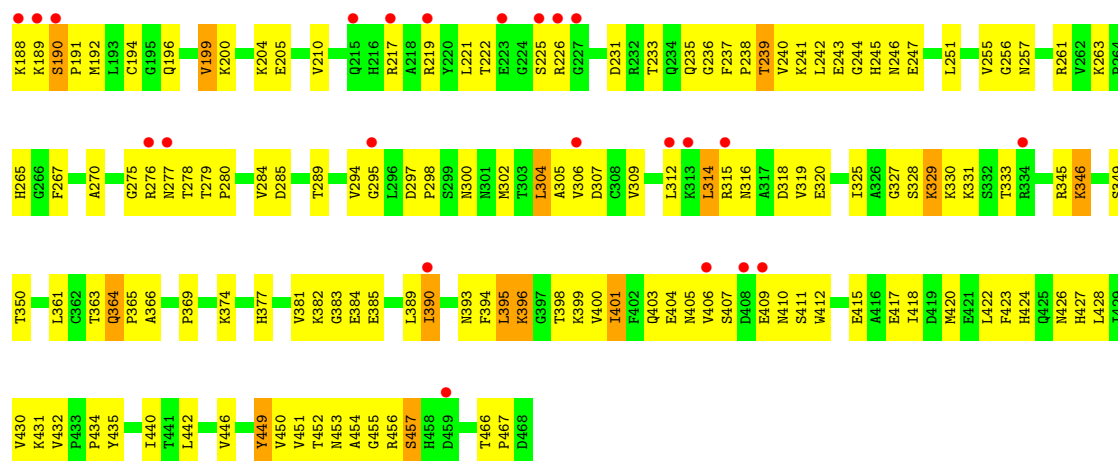


- Molecule 3: NUCLEAR FACTOR OF ACTIVATED T CELLS 5



- Molecule 3: NUCLEAR FACTOR OF ACTIVATED T CELLS 5





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	59.57Å 95.37Å 158.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.50 – 2.86 29.50 – 2.86	Depositor EDS
% Data completeness (in resolution range)	87.5 (29.50-2.86) 94.7 (29.50-2.86)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 2.85Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.244 , 0.290 0.241 , 0.283	Depositor DCC
R_{free} test set	1358 reflections (6.44%)	wwPDB-VP
Wilson B-factor (Å ²)	68.4	Xtriage
Anisotropy	0.285	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 55.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4977	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% 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

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	0.43	0/349	0.78	0/538
2	B	0.42	0/333	1.00	0/511
3	C	0.45	0/2226	1.03	8/3012 (0.3%)
3	D	0.43	0/2226	0.98	9/3012 (0.3%)
All	All	0.44	0/5134	0.99	17/7073 (0.2%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	366	ALA	N-CA-C	8.61	120.67	111.28
3	C	364	GLN	CA-C-N	8.44	128.50	119.89
3	C	364	GLN	C-N-CA	8.44	128.50	119.89
3	C	411	SER	N-CA-C	-7.01	102.13	110.41
3	C	362	CYS	N-CA-C	6.61	120.33	112.93
3	D	331	LYS	N-CA-C	6.17	119.57	109.76
3	C	328	SER	N-CA-C	-5.76	105.51	112.54
3	C	331	LYS	N-CA-C	-5.69	98.06	108.02
3	D	325	ILE	N-CA-C	5.62	115.81	110.42
3	C	401	ILE	N-CA-C	5.49	115.77	107.75
3	D	401	ILE	N-CA-C	5.44	115.69	107.75
3	D	309	VAL	N-CA-C	5.37	115.63	108.11
3	D	329	LYS	N-CA-C	-5.28	106.89	113.55
3	D	226	ARG	CA-C-N	-5.28	115.86	121.45
3	D	226	ARG	C-N-CA	-5.28	115.86	121.45
3	D	364	GLN	CA-C-N	5.00	126.09	119.84
3	D	364	GLN	C-N-CA	5.00	126.09	119.84

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	310	0	171	30	0
2	B	299	0	173	22	0
3	C	2184	0	2213	134	0
3	D	2184	0	2213	133	0
All	All	4977	0	4770	312	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 32.

All (312) 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:4004:DC:H2''	1:A:4005:DT:H5''	1.32	1.09
3:D:400:VAL:HG21	3:D:430:VAL:HG11	1.38	1.05
3:C:400:VAL:HG21	3:C:430:VAL:HG11	1.40	1.02
1:A:4007:DG:H2''	1:A:4008:DA:H5''	1.39	1.01
3:C:451:VAL:HG12	3:C:456:ARG:HG2	1.45	0.99
3:D:407:SER:HB3	3:D:411:SER:HB3	1.44	0.98
3:D:451:VAL:HG12	3:D:456:ARG:HG2	1.46	0.96
3:C:396:LYS:HA	3:C:396:LYS:HE3	1.47	0.95
3:D:396:LYS:HE3	3:D:396:LYS:HA	1.48	0.94
1:A:4005:DT:H2''	1:A:4006:DG:C8	2.09	0.86
3:D:346:LYS:HE3	3:D:346:LYS:HA	1.58	0.85
1:A:4004:DC:C2'	1:A:4005:DT:H5''	2.06	0.83
3:C:407:SER:HB3	3:C:411:SER:HB3	1.58	0.83
1:A:4007:DG:C2'	1:A:4008:DA:H5''	2.09	0.83
3:C:346:LYS:HE3	3:C:346:LYS:HA	1.59	0.83
1:A:4007:DG:H2''	1:A:4008:DA:C5'	2.10	0.81
3:D:381:VAL:HG13	3:D:435:TYR:HB3	1.63	0.81
3:C:409:GLU:O	3:C:410:ASN:HB2	1.81	0.80
3:C:381:VAL:HG13	3:C:435:TYR:HB3	1.63	0.80
3:C:196:GLN:HE22	3:C:261:ARG:HH11	1.32	0.77
1:A:4013:DT:H2''	1:A:4014:DA:H5''	1.66	0.77
3:D:315:ARG:HG2	3:D:318:ASP:OD2	1.84	0.77
3:C:189:LYS:HE3	3:C:191:PRO:HG3	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:221:LEU:HD23	3:D:221:LEU:O	1.85	0.76
3:C:239:THR:HG23	3:C:305:ALA:HA	1.67	0.76
3:D:297:ASP:CG	3:D:298:PRO:HD2	2.10	0.76
3:D:239:THR:HG23	3:D:305:ALA:HA	1.67	0.75
3:C:297:ASP:CG	3:C:298:PRO:HD2	2.12	0.75
3:D:196:GLN:HE22	3:D:261:ARG:HH11	1.34	0.74
1:A:4001:DT:H2''	1:A:4002:DT:OP2	1.87	0.74
3:D:297:ASP:OD1	3:D:298:PRO:HD2	1.89	0.73
2:B:5003:DC:H2'	2:B:5004:DT:H71	1.69	0.73
3:D:189:LYS:HE3	3:D:191:PRO:HG3	1.69	0.73
3:C:404:GLU:HB2	3:C:411:SER:O	1.90	0.72
3:C:297:ASP:OD1	3:C:298:PRO:HD2	1.89	0.72
1:A:4008:DA:H2''	1:A:4009:DA:C8	2.26	0.70
3:C:200:LYS:HB3	3:C:205:GLU:HG3	1.72	0.70
3:D:200:LYS:HB3	3:D:205:GLU:HG3	1.72	0.70
1:A:4012:DA:H1'	1:A:4013:DT:H5''	1.74	0.69
1:A:4004:DC:H2''	1:A:4005:DT:C5'	2.17	0.69
3:C:220:TYR:CZ	3:C:313:LYS:HG2	2.27	0.68
2:B:5011:DC:H2''	2:B:5012:DC:H5'	1.75	0.68
3:C:204:LYS:HG2	3:C:244:GLY:O	1.94	0.67
1:A:4013:DT:C2'	1:A:4014:DA:H5''	2.24	0.67
1:A:4013:DT:H2''	1:A:4014:DA:C5'	2.25	0.66
3:D:204:LYS:HG2	3:D:244:GLY:O	1.94	0.66
3:D:403:GLN:O	3:D:446:VAL:HB	1.94	0.66
3:C:219:ARG:HD2	3:C:224:GLY:O	1.95	0.66
3:C:383:GLY:O	3:C:384:GLU:HB2	1.96	0.66
3:C:403:GLN:O	3:C:446:VAL:HB	1.96	0.66
3:D:399:LYS:HB2	3:D:451:VAL:CG2	2.26	0.65
3:C:399:LYS:HB2	3:C:451:VAL:CG2	2.27	0.64
3:C:329:LYS:O	3:C:330:LYS:HB3	1.97	0.64
2:B:5001:DA:HO5'	2:B:5001:DA:H8	1.44	0.64
3:C:452:THR:HG23	3:C:454:ALA:H	1.63	0.64
3:D:219:ARG:O	3:D:312:LEU:HD12	1.95	0.64
3:C:396:LYS:HA	3:C:396:LYS:CE	2.27	0.64
3:C:381:VAL:HG23	3:C:466:THR:O	1.97	0.64
3:C:389:LEU:HD12	3:C:428:LEU:HD11	1.81	0.63
3:D:245:HIS:HE2	3:D:247:GLU:HB2	1.63	0.63
3:D:381:VAL:HG23	3:D:466:THR:O	1.96	0.63
3:C:189:LYS:HD2	3:C:189:LYS:O	1.97	0.63
3:C:245:HIS:HE2	3:C:247:GLU:HB2	1.62	0.63
3:D:383:GLY:O	3:D:384:GLU:HB2	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:389:LEU:HD12	3:D:428:LEU:HD11	1.81	0.62
3:D:452:THR:HG23	3:D:454:ALA:H	1.63	0.62
3:D:189:LYS:HD2	3:D:189:LYS:O	1.98	0.62
3:D:190:SER:N	3:D:191:PRO:HD3	2.15	0.62
3:C:189:LYS:HG3	3:C:350:THR:HG21	1.82	0.61
3:D:219:ARG:HD2	3:D:225:SER:O	2.01	0.61
3:D:267:PHE:CE1	3:D:319:VAL:HG11	2.36	0.61
3:D:304:LEU:HD22	3:D:305:ALA:N	2.15	0.61
3:D:242:LEU:HD23	3:D:302:MET:HE3	1.83	0.61
3:D:221:LEU:HD23	3:D:221:LEU:C	2.25	0.60
3:C:190:SER:N	3:C:191:PRO:HD3	2.16	0.60
3:D:189:LYS:HG3	3:D:350:THR:HG21	1.82	0.60
3:D:405:ASN:ND2	3:D:406:VAL:H	1.99	0.60
1:A:4011:DA:H2''	1:A:4012:DA:H5''	1.84	0.60
3:C:418:ILE:HG12	3:C:430:VAL:HG12	1.84	0.60
3:C:304:LEU:HD22	3:C:305:ALA:N	2.17	0.60
3:C:278:THR:HA	3:C:307:ASP:OD2	2.02	0.59
3:D:424:HIS:HE1	3:D:426:ASN:HD22	1.50	0.59
3:C:242:LEU:HD23	3:C:302:MET:HE3	1.85	0.59
1:A:4011:DA:H2''	1:A:4012:DA:C5'	2.33	0.59
3:D:452:THR:C	3:D:454:ALA:H	2.11	0.59
3:C:245:HIS:CD2	3:C:247:GLU:H	2.21	0.59
3:D:396:LYS:HA	3:D:396:LYS:CE	2.27	0.59
3:C:345:ARG:NH1	3:C:349:SER:HB2	2.18	0.59
3:D:245:HIS:CD2	3:D:247:GLU:H	2.20	0.59
3:C:256:GLY:HA2	3:C:265:HIS:H	1.68	0.58
3:D:278:THR:HA	3:D:307:ASP:OD2	2.02	0.58
3:C:385:GLU:O	3:C:432:VAL:HG23	2.04	0.58
2:B:5006:DT:H2''	2:B:5007:DT:H5'	1.85	0.58
3:D:418:ILE:HG12	3:D:430:VAL:HG12	1.83	0.58
3:C:245:HIS:HD2	3:C:247:GLU:H	1.52	0.58
3:D:239:THR:HG23	3:D:305:ALA:CA	2.34	0.58
3:C:452:THR:C	3:C:454:ALA:H	2.10	0.58
3:D:210:VAL:O	3:D:238:PRO:HA	2.03	0.58
1:A:4011:DA:C2'	1:A:4012:DA:H5''	2.34	0.57
3:D:369:PRO:HD3	3:D:452:THR:HG21	1.86	0.57
3:C:424:HIS:HE1	3:C:426:ASN:HD22	1.52	0.57
3:D:404:GLU:HB2	3:D:411:SER:O	2.03	0.57
3:D:256:GLY:HA2	3:D:265:HIS:H	1.68	0.57
3:C:382:LYS:O	3:C:434:PRO:HB3	2.05	0.57
3:D:221:LEU:N	3:D:312:LEU:HD11	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:345:ARG:NH1	3:D:349:SER:HB2	2.18	0.57
3:C:239:THR:HG23	3:C:305:ALA:CA	2.33	0.57
3:D:382:LYS:O	3:D:434:PRO:HB3	2.04	0.57
2:B:5012:DC:H2''	2:B:5013:DA:C8	2.40	0.56
3:D:235:GLN:OE1	3:D:235:GLN:HA	2.04	0.56
3:D:385:GLU:O	3:D:432:VAL:HG23	2.04	0.56
1:A:4005:DT:H2''	1:A:4006:DG:H8	1.69	0.56
3:C:401:ILE:HB	3:C:449:TYR:CE2	2.40	0.56
3:C:369:PRO:HD3	3:C:452:THR:HG21	1.87	0.56
3:D:245:HIS:HD2	3:D:247:GLU:H	1.51	0.56
1:A:4011:DA:H1'	1:A:4012:DA:H5''	1.88	0.56
3:D:196:GLN:HE22	3:D:261:ARG:NH1	2.04	0.56
3:C:325:ILE:O	3:C:329:LYS:HB2	2.06	0.56
1:A:4008:DA:H62	3:C:364:GLN:HE22	1.53	0.55
3:C:452:THR:O	3:C:454:ALA:N	2.39	0.55
3:C:330:LYS:HG3	3:C:330:LYS:O	2.05	0.55
2:B:5002:DA:H1'	2:B:5003:DC:H5''	1.87	0.55
3:C:210:VAL:O	3:C:238:PRO:HA	2.06	0.55
3:D:369:PRO:HD3	3:D:452:THR:CG2	2.36	0.55
3:D:401:ILE:HB	3:D:449:TYR:CE2	2.41	0.55
3:D:452:THR:O	3:D:454:ALA:N	2.40	0.55
3:C:235:GLN:HA	3:C:235:GLN:OE1	2.05	0.55
3:C:257:ASN:ND2	3:C:263:LYS:HB2	2.22	0.55
1:A:4010:DA:H2''	1:A:4011:DA:OP2	2.06	0.55
3:D:440:ILE:HD12	3:D:442:LEU:O	2.07	0.54
3:D:452:THR:C	3:D:454:ALA:N	2.64	0.54
3:C:440:ILE:HD12	3:C:442:LEU:O	2.07	0.54
3:D:257:ASN:ND2	3:D:263:LYS:HB2	2.22	0.54
2:B:5011:DC:H2''	2:B:5012:DC:C5'	2.37	0.54
3:C:395:LEU:O	3:C:398:THR:HG23	2.08	0.54
3:C:423:PHE:CD1	3:C:424:HIS:N	2.76	0.54
3:C:196:GLN:HE22	3:C:261:ARG:NH1	2.02	0.54
3:C:398:THR:HA	3:C:451:VAL:O	2.08	0.54
3:C:369:PRO:HD3	3:C:452:THR:CG2	2.37	0.53
3:D:423:PHE:CD1	3:D:424:HIS:N	2.77	0.53
2:B:5001:DA:H8	2:B:5001:DA:O5'	1.91	0.53
3:D:398:THR:HA	3:D:451:VAL:O	2.08	0.53
2:B:5003:DC:H2''	2:B:5004:DT:C6	2.44	0.53
2:B:5003:DC:C2'	2:B:5004:DT:H71	2.36	0.53
3:D:327:GLY:C	3:D:329:LYS:H	2.17	0.53
3:C:395:LEU:HD23	3:C:452:THR:OG1	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:255:VAL:HG23	3:C:270:ALA:HB2	1.91	0.52
3:D:251:LEU:HB3	3:D:294:VAL:CG1	2.39	0.52
3:D:346:LYS:HE3	3:D:346:LYS:CA	2.34	0.52
3:D:217:ARG:HD2	3:D:364:GLN:HG3	1.91	0.52
3:C:275:GLY:C	3:C:277:ASN:H	2.17	0.52
3:D:237:PHE:HB3	3:D:238:PRO:HD2	1.92	0.52
2:B:5006:DT:H1'	2:B:5007:DT:H5''	1.92	0.52
3:C:345:ARG:HB2	3:C:349:SER:OG	2.10	0.52
3:D:275:GLY:C	3:D:277:ASN:H	2.17	0.52
3:D:327:GLY:O	3:D:330:LYS:HG2	2.10	0.52
3:D:189:LYS:O	3:D:190:SER:OG	2.26	0.52
3:C:346:LYS:HE3	3:C:346:LYS:CA	2.35	0.51
3:D:395:LEU:O	3:D:398:THR:HG23	2.09	0.51
3:D:284:VAL:HG22	3:D:285:ASP:N	2.25	0.51
3:D:384:GLU:OE1	3:D:384:GLU:HA	2.10	0.51
3:D:405:ASN:CG	3:D:406:VAL:H	2.17	0.51
3:D:345:ARG:HB2	3:D:349:SER:OG	2.09	0.51
3:C:251:LEU:HB3	3:C:294:VAL:CG1	2.40	0.51
3:C:407:SER:CB	3:C:411:SER:HB3	2.34	0.51
3:D:390:ILE:HD12	3:D:390:ILE:C	2.35	0.51
3:D:405:ASN:ND2	3:D:406:VAL:N	2.58	0.51
3:D:255:VAL:HG23	3:D:270:ALA:HB2	1.92	0.50
3:C:325:ILE:O	3:C:325:ILE:HG22	2.12	0.50
3:D:251:LEU:HB3	3:D:294:VAL:HG13	1.94	0.50
3:C:403:GLN:NE2	3:C:405:ASN:O	2.45	0.50
3:C:452:THR:C	3:C:454:ALA:N	2.64	0.50
3:C:261:ARG:NH1	3:C:261:ARG:HB3	2.27	0.50
3:C:284:VAL:HG22	3:C:285:ASP:N	2.26	0.50
3:C:422:LEU:HD13	3:D:390:ILE:HD11	1.93	0.50
3:C:390:ILE:C	3:C:390:ILE:HD12	2.36	0.50
3:C:346:LYS:HA	3:C:346:LYS:CE	2.39	0.49
3:D:261:ARG:HH11	3:D:261:ARG:HB3	1.76	0.49
3:C:440:ILE:HG13	3:C:467:PRO:HG3	1.94	0.49
3:D:261:ARG:NH1	3:D:261:ARG:HB3	2.27	0.49
1:A:4012:DA:H2''	1:A:4013:DT:C5'	2.42	0.49
3:C:384:GLU:HA	3:C:384:GLU:OE1	2.11	0.49
3:D:395:LEU:HD23	3:D:452:THR:OG1	2.10	0.49
2:B:5005:DA:H1'	2:B:5006:DT:H5''	1.93	0.49
3:C:200:LYS:HA	3:C:204:LYS:O	2.12	0.49
3:D:304:LEU:HD22	3:D:305:ALA:H	1.78	0.49
3:D:346:LYS:HA	3:D:346:LYS:CE	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4006:DG:H2''	1:A:4007:DG:H5'	1.95	0.49
3:C:452:THR:HG23	3:C:455:GLY:H	1.78	0.49
3:C:241:LYS:HE3	3:C:243:GLU:HG2	1.94	0.49
3:D:409:GLU:O	3:D:410:ASN:HB2	2.13	0.49
3:C:428:LEU:HD12	3:C:428:LEU:O	2.13	0.48
3:C:219:ARG:CD	3:C:225:SER:HA	2.44	0.48
3:C:237:PHE:HB3	3:C:238:PRO:HD2	1.95	0.48
3:C:261:ARG:HH11	3:C:261:ARG:HB3	1.77	0.48
3:C:401:ILE:HD11	3:C:415:GLU:HG2	1.96	0.48
3:D:401:ILE:HD11	3:D:415:GLU:HG2	1.95	0.48
3:D:241:LYS:HE3	3:D:243:GLU:HG2	1.95	0.48
3:C:374:LYS:HE2	3:C:377:HIS:CD2	2.49	0.48
3:C:219:ARG:NH1	3:C:220:TYR:O	2.47	0.48
3:D:200:LYS:HA	3:D:204:LYS:O	2.13	0.48
3:D:452:THR:HG23	3:D:455:GLY:H	1.78	0.48
3:C:369:PRO:HG2	3:C:457:SER:N	2.30	0.47
3:D:374:LYS:HE2	3:D:377:HIS:CD2	2.49	0.47
3:D:440:ILE:HG13	3:D:467:PRO:HG3	1.95	0.47
2:B:5001:DA:O5'	2:B:5001:DA:C8	2.65	0.47
3:D:190:SER:N	3:D:191:PRO:CD	2.77	0.47
3:C:452:THR:CG2	3:C:455:GLY:H	2.28	0.47
3:C:251:LEU:HB3	3:C:294:VAL:HG13	1.95	0.47
2:B:5009:DT:OP2	3:C:313:LYS:HE2	2.15	0.47
3:C:231:ASP:OD2	3:C:233:THR:OG1	2.33	0.47
1:A:4006:DG:H1'	1:A:4007:DG:H5''	1.97	0.46
3:C:304:LEU:HD22	3:C:305:ALA:H	1.80	0.46
3:D:247:GLU:O	3:D:302:MET:HE1	2.15	0.46
3:C:394:PHE:HA	3:C:398:THR:HG21	1.98	0.46
3:D:428:LEU:O	3:D:428:LEU:HD12	2.15	0.46
3:C:189:LYS:O	3:C:190:SER:OG	2.27	0.46
3:C:390:ILE:HD11	3:D:422:LEU:HD13	1.98	0.46
3:D:315:ARG:O	3:D:316:ASN:C	2.59	0.46
3:D:403:GLN:NE2	3:D:405:ASN:O	2.48	0.46
3:D:394:PHE:HA	3:D:398:THR:HG21	1.98	0.45
3:D:452:THR:CG2	3:D:455:GLY:H	2.28	0.45
1:A:4012:DA:C1'	1:A:4013:DT:H5''	2.44	0.45
3:C:190:SER:N	3:C:191:PRO:CD	2.79	0.45
3:C:219:ARG:NH1	3:C:223:GLU:O	2.49	0.45
3:C:247:GLU:O	3:C:302:MET:HE1	2.16	0.45
3:C:298:PRO:C	3:C:300:ASN:N	2.75	0.45
3:C:401:ILE:CD1	3:C:415:GLU:HG2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:383:GLY:O	3:C:384:GLU:CB	2.64	0.45
3:C:428:LEU:HD12	3:C:428:LEU:C	2.42	0.45
3:D:417:GLU:OE1	3:D:431:LYS:HE2	2.17	0.45
3:C:346:LYS:CA	3:C:346:LYS:CE	2.95	0.44
3:D:346:LYS:CA	3:D:346:LYS:CE	2.94	0.44
3:D:401:ILE:CD1	3:D:415:GLU:HG2	2.46	0.44
3:C:417:GLU:OE1	3:C:431:LYS:HE2	2.17	0.44
3:D:199:VAL:HG13	3:D:200:LYS:N	2.32	0.44
3:D:298:PRO:C	3:D:300:ASN:N	2.75	0.44
3:D:316:ASN:O	3:D:320:GLU:HG3	2.18	0.44
3:C:256:GLY:HA2	3:C:265:HIS:N	2.31	0.44
3:C:316:ASN:O	3:C:319:VAL:N	2.50	0.44
3:C:364:GLN:HA	3:C:365:PRO:HD3	1.82	0.44
3:D:221:LEU:C	3:D:221:LEU:CD2	2.90	0.44
3:D:369:PRO:HG2	3:D:457:SER:N	2.32	0.44
3:C:345:ARG:HH11	3:C:349:SER:CB	2.31	0.44
2:B:5007:DT:H2''	2:B:5008:DT:H5'	1.99	0.44
3:C:409:GLU:HA	3:C:409:GLU:OE1	2.17	0.43
3:D:364:GLN:HA	3:D:365:PRO:HD3	1.75	0.43
2:B:5003:DC:H2'	2:B:5004:DT:C7	2.45	0.43
2:B:5007:DT:H2'	2:B:5008:DT:H72	2.00	0.43
3:C:330:LYS:O	3:C:330:LYS:CG	2.66	0.43
3:D:428:LEU:HD12	3:D:428:LEU:C	2.44	0.43
1:A:4013:DT:H1'	1:A:4014:DA:H5''	2.01	0.43
1:A:4012:DA:C2'	1:A:4013:DT:H5''	2.48	0.43
3:D:400:VAL:HG21	3:D:430:VAL:CG1	2.29	0.43
3:C:199:VAL:HG13	3:C:200:LYS:N	2.33	0.43
3:C:294:VAL:HG22	3:C:295:GLY:N	2.34	0.43
3:C:325:ILE:O	3:C:329:LYS:CB	2.67	0.43
3:D:256:GLY:HA2	3:D:265:HIS:N	2.31	0.43
3:D:383:GLY:O	3:D:384:GLU:CB	2.64	0.42
2:B:5007:DT:H1'	2:B:5008:DT:H5'	2.00	0.42
3:D:251:LEU:HD23	3:D:294:VAL:HG11	2.00	0.42
3:D:315:ARG:CG	3:D:318:ASP:OD2	2.61	0.42
3:C:192:MET:HE2	3:C:195:GLY:HA2	2.02	0.42
3:D:245:HIS:NE2	3:D:247:GLU:HB2	2.33	0.42
3:D:345:ARG:HH11	3:D:349:SER:CB	2.33	0.42
3:D:400:VAL:HA	3:D:450:VAL:HG12	2.00	0.42
3:D:237:PHE:CD2	3:D:307:ASP:HA	2.55	0.42
3:D:267:PHE:O	3:D:314:LEU:HB2	2.19	0.42
2:B:5008:DT:H1'	2:B:5009:DT:H5'	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:245:HIS:NE2	3:C:247:GLU:HB2	2.32	0.42
3:C:256:GLY:HA2	3:C:264:PRO:HA	2.02	0.42
3:C:381:VAL:HG12	3:C:438:GLN:OE1	2.19	0.42
3:C:461:GLN:HA	3:C:462:PRO:HD3	1.84	0.42
1:A:4003:DG:H2''	1:A:4004:DC:OP2	2.20	0.42
3:D:333:THR:HB	3:D:363:THR:HG23	2.01	0.42
2:B:5002:DA:N7	3:D:225:SER:HB2	2.35	0.42
3:C:231:ASP:OD1	3:C:236:GLY:N	2.53	0.42
3:D:420:MET:C	3:D:422:LEU:H	2.28	0.42
3:C:427:HIS:CD2	3:C:427:HIS:C	2.98	0.42
3:C:240:VAL:HG11	3:C:251:LEU:HD21	2.01	0.41
3:C:345:ARG:NH1	3:C:349:SER:CB	2.83	0.41
3:D:330:LYS:O	3:D:330:LYS:HG3	2.19	0.41
3:D:294:VAL:HG22	3:D:295:GLY:N	2.35	0.41
3:D:381:VAL:CG1	3:D:435:TYR:HB3	2.42	0.41
3:D:393:ASN:O	3:D:395:LEU:HD22	2.19	0.41
3:C:315:ARG:O	3:C:318:ASP:HB2	2.20	0.41
3:D:192:MET:HE3	3:D:194:CYS:HB2	2.03	0.41
3:D:279:THR:HG23	3:D:280:PRO:HD2	2.02	0.41
2:B:5006:DT:H2''	2:B:5007:DT:C5'	2.51	0.41
3:C:192:MET:HE3	3:C:194:CYS:HB2	2.02	0.41
3:C:237:PHE:CD2	3:C:307:ASP:HA	2.55	0.41
3:C:452:THR:HG23	3:C:455:GLY:N	2.35	0.41
3:D:315:ARG:O	3:D:318:ASP:N	2.46	0.41
1:A:4013:DT:OP2	3:D:222:THR:CG2	2.69	0.41
2:B:5004:DT:H2''	2:B:5005:DA:OP2	2.21	0.41
3:C:233:THR:C	3:C:235:GLN:H	2.28	0.41
3:C:251:LEU:HD23	3:C:294:VAL:HG11	2.02	0.41
3:C:400:VAL:HA	3:C:450:VAL:HG12	2.01	0.41
3:D:240:VAL:HG11	3:D:251:LEU:HD21	2.03	0.41
3:D:427:HIS:CD2	3:D:427:HIS:C	2.98	0.41
3:D:452:THR:HG23	3:D:455:GLY:N	2.35	0.41
1:A:4011:DA:C1'	1:A:4012:DA:H5''	2.51	0.41
3:C:316:ASN:O	3:C:317:ALA:C	2.63	0.41
3:C:403:GLN:HG3	3:C:413:LYS:HG2	2.03	0.41
3:D:231:ASP:OD2	3:D:233:THR:OG1	2.38	0.41
3:C:374:LYS:HA	3:C:388:PHE:O	2.21	0.40
3:C:400:VAL:HG21	3:C:430:VAL:CG1	2.30	0.40
3:D:231:ASP:OD1	3:D:236:GLY:N	2.54	0.40
3:C:267:PHE:O	3:C:314:LEU:HB2	2.21	0.40
1:A:4013:DT:P	3:D:222:THR:HG21	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:395:LEU:N	3:C:398:THR:CG2	2.85	0.40
3:C:399:LYS:HB2	3:C:451:VAL:HG23	2.02	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	
3	C	279/281 (99%)	240 (86%)	31 (11%)	8 (3%)	3	8
3	D	279/281 (99%)	247 (88%)	24 (9%)	8 (3%)	3	8
All	All	558/562 (99%)	487 (87%)	55 (10%)	16 (3%)	3	8

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	410	ASN
3	D	412	TRP
3	C	330	LYS
3	C	457	SER
3	C	276	ARG
3	C	412	TRP
3	C	453	ASN
3	D	276	ARG
3	D	453	ASN
3	D	457	SER
3	D	328	SER
3	D	366	ALA
3	D	190	SER
3	C	190	SER
3	C	306	VAL
3	D	306	VAL

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	
3	C	249/249 (100%)	235 (94%)	14 (6%)	19	40
3	D	249/249 (100%)	236 (95%)	13 (5%)	21	43
All	All	498/498 (100%)	471 (95%)	27 (5%)	20	42

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	188	LYS
3	C	199	VAL
3	C	225	SER
3	C	239	THR
3	C	246	ASN
3	C	289	THR
3	C	304	LEU
3	C	314	LEU
3	C	346	LYS
3	C	361	LEU
3	C	390	ILE
3	C	395	LEU
3	C	396	LYS
3	C	449	TYR
3	D	188	LYS
3	D	199	VAL
3	D	239	THR
3	D	246	ASN
3	D	289	THR
3	D	304	LEU
3	D	314	LEU
3	D	346	LYS
3	D	361	LEU
3	D	390	ILE
3	D	395	LEU
3	D	396	LYS
3	D	449	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	196	GLN
3	C	215	GLN
3	C	252	GLN
3	C	300	ASN
3	C	342	ASN
3	C	364	GLN
3	C	377	HIS
3	C	393	ASN
3	C	405	ASN
3	C	426	ASN
3	D	196	GLN
3	D	252	GLN
3	D	300	ASN
3	D	377	HIS
3	D	393	ASN
3	D	405	ASN
3	D	426	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	15/15 (100%)	0.27	1 (6%) 24 17	28, 46, 72, 82	0
2	B	15/15 (100%)	-0.11	0 100 100	28, 44, 62, 74	0
3	C	281/281 (100%)	0.51	19 (6%) 23 17	28, 70, 104, 127	0
3	D	281/281 (100%)	0.61	23 (8%) 17 13	27, 72, 100, 122	0
All	All	592/592 (100%)	0.54	43 (7%) 21 15	27, 70, 103, 127	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	326	ALA	5.0
3	C	325	ILE	4.2
3	D	408	ASP	4.0
3	C	453	ASN	3.7
3	D	219	ARG	3.6
3	D	189	LYS	3.4
3	D	313	LYS	3.4
3	C	189	LYS	3.3
3	C	454	ALA	3.3
3	C	409	GLU	3.2
3	D	223	GLU	3.1
1	A	4001	DT	3.1
3	D	277	ASN	3.0
3	D	226	ARG	2.9
3	D	409	GLU	2.9
3	C	330	LYS	2.9
3	D	227	GLY	2.8
3	D	315	ARG	2.7
3	D	406	VAL	2.6
3	C	458	HIS	2.6
3	C	323	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
3	D	188	LYS	2.4
3	C	271	CYS	2.4
3	D	312	LEU	2.4
3	C	324	GLY	2.3
3	D	225	SER	2.3
3	C	322	ARG	2.3
3	C	327	GLY	2.3
3	C	188	LYS	2.3
3	C	406	VAL	2.3
3	D	295	GLY	2.2
3	D	276	ARG	2.2
3	D	215	GLN	2.2
3	C	250	VAL	2.2
3	D	190	SER	2.2
3	D	306	VAL	2.1
3	D	217	ARG	2.1
3	D	334	ARG	2.1
3	D	390	ILE	2.1
3	C	331	LYS	2.1
3	D	459	ASP	2.1
3	C	202	GLU	2.1
3	C	449	TYR	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.