



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 04:37 am BST

PDB ID : 1IMH
Title : TonEBP/DNA COMPLEX
Authors : Stroud, J.C.; Lopez-Rodriguez, C.; Rao, A.; Chen, L.
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

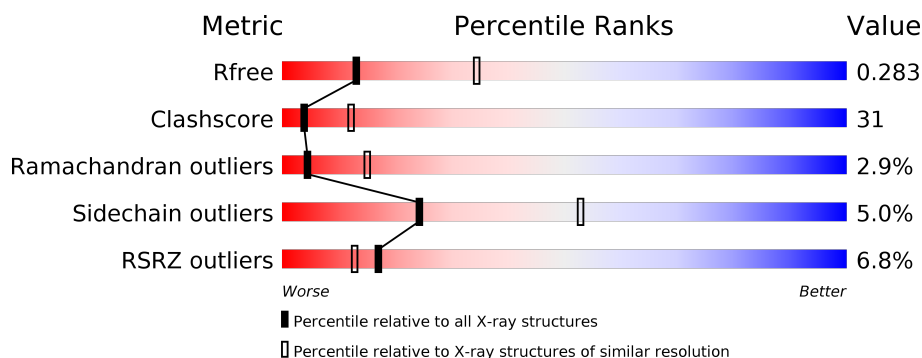
1 Overall quality at a glance

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}	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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 on 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	<div> <div>7%</div> <div>7%</div> <div>93%</div> </div>
2	B	15	<div> <div>20%</div> <div>80%</div> </div>
3	C	281	<div> <div>9%</div> <div>54%</div> <div>42%</div> <div>5%</div> </div>
3	D	281	<div> <div>5%</div> <div>53%</div> <div>43%</div> <div>.</div> </div>

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 [i](#)

These plots are drawn for all protein, RNA and DNA 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.

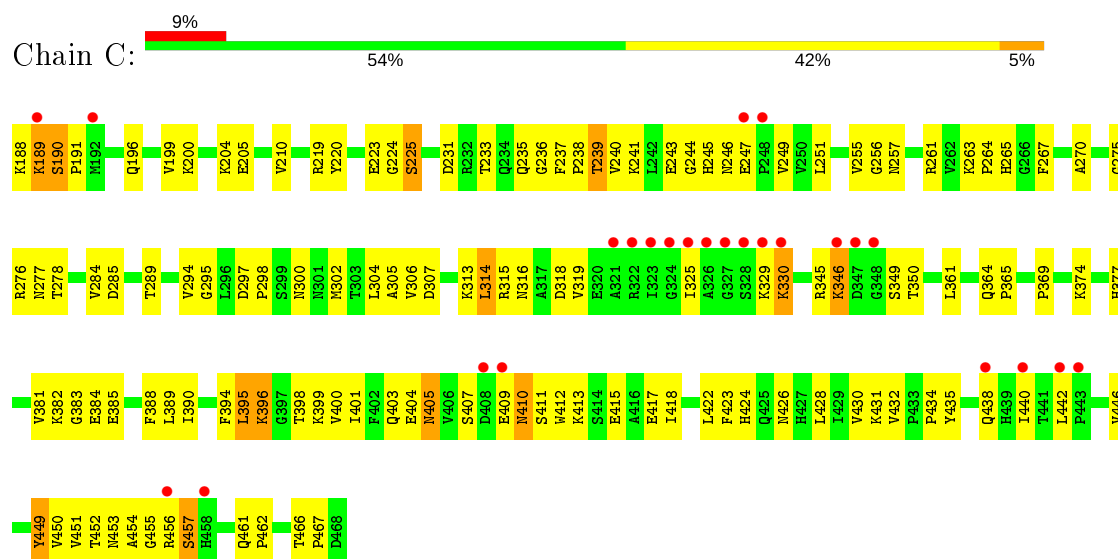
- Molecule 1: 5'-D(*TP*TP*GP*CP*TP*GP*GP*AP*AP*AP*AP*AP*TP*AP*G)-3'



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

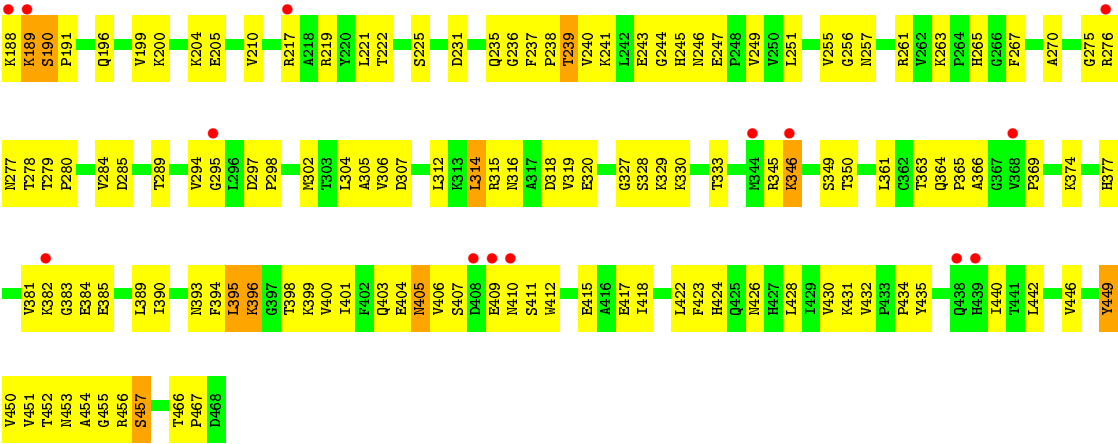


- Molecule 3: NUCLEAR FACTOR OF ACTIVATED T CELLS 5



- 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) 94.8 (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 , 58.8	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 [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	0.68	0/349	0.79	0/538
2	B	0.66	0/333	0.90	0/511
3	C	0.37	0/2226	0.67	0/3012
3	D	0.36	0/2226	0.65	0/3012
All	All	0.42	0/5134	0.69	0/7073

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	20	0
3	C	2184	0	2213	128	0
3	D	2184	0	2213	126	0
All	All	4977	0	4770	297	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 31.

All (297) 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:HA	3:D:396:LYS:HE3	1.48	0.94
1:A:4005:DT:H2''	1:A:4006:DG:C8	2.09	0.86
3:D:346:LYS:HA	3:D:346:LYS:HE3	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:HA	3:C:346:LYS:HE3	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
3:D:221:LEU:O	3:D:221:LEU:HD23	1.85	0.76
3:C:239:THR:HG23	3:C:305:ALA:HA	1.67	0.76
3:D:239:THR:HG23	3:D:305:ALA:HA	1.67	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
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
3:D:297:ASP:CG	3:D:298:PRO:HD2	2.10	0.71
1:A:4008:DA:H2''	1:A:4009:DA:C8	2.26	0.70
2:B:5003:DC:H2'	2:B:5004:DT:H72	1.73	0.70
3:C:200:LYS:HB3	3:C:205:GLU:HG3	1.72	0.70
3:C:297:ASP:CG	3:C:298:PRO:HD2	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:383:GLY:O	3:D:384:GLU:HB2	1.97	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:CE	3:C:396:LYS:HA	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:O	3:C:189:LYS:HD2	1.97	0.63
3:C:245:HIS:HE2	3:C:247:GLU:HB2	1.62	0.63
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:O	3:D:189:LYS:HD2	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: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
1:A:4011:DA:H2''	1:A:4012:DA:C5'	2.33	0.59
3:C:245:HIS:CD2	3:C:247:GLU:H	2.21	0.59
3:D:396:LYS:CE	3:D:396:LYS:HA	2.27	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
3:D:221:LEU:HD23	3:D:221:LEU:C	2.25	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:O	3:C:330:LYS:HG3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
3:D:452:THR:C	3:D:454:ALA:H	2.11	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:C:452:THR:C	3:C:454:ALA:H	2.10	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
3:C:395:LEU:HD23	3:C:452:THR:OG1	2.09	0.53
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:CA	3:D:346:LYS:HE3	2.34	0.52
3:D:217:ARG:HD2	3:D:364:GLN:HG3	1.91	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:327:GLY:O	3:D:330:LYS:HG2	2.10	0.52
3:C:452:THR:C	3:C:454:ALA:N	2.64	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:HA	3:D:384:GLU:OE1	2.10	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:452:THR:C	3:D:454:ALA:N	2.64	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:261:ARG:NH1	3:C:261:ARG:HB3	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:346:LYS:CE	3:C:346:LYS:HA	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:HB3	3:D:261:ARG:NH1	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
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:O	3:C:428:LEU:HD12	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:HB3	3:C:261:ARG:HH11	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:D:327:GLY:C	3:D:329:LYS:H	2.17	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:275:GLY:C	3:C:277:ASN:H	2.17	0.47
3:C:369:PRO:HG2	3:C:457:SER:N	2.30	0.47
3:D:275:GLY:C	3:D:277:ASN:H	2.17	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:C8	2:B:5001:DA:O5'	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:D:405:ASN:CG	3:D:406:VAL:H	2.17	0.47
1:A:4006:DG:H1'	1:A:4007:DG:H5''	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:304:LEU:HD22	3:C:305:ALA:H	1.80	0.46
3:C:394:PHE:HA	3:C:398:THR:HG21	1.98	0.46
3:D:390:ILE:HD12	3:D:390:ILE:C	2.35	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: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:390:ILE:HD12	3:C:390:ILE:C	2.36	0.45
3:C:401:ILE:CD1	3:C:415:GLU:HG2	2.46	0.45
3:C:383:GLY:O	3:C:384:GLU:CB	2.64	0.45
3:D:247:GLU:O	3:D:302:MET:HE1	2.17	0.45
3:D:417:GLU:OE1	3:D:431:LYS:HE2	2.17	0.45
3:C:346:LYS:CE	3:C:346:LYS:CA	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: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:369:PRO:HG2	3:D:457:SER:N	2.32	0.44
3:D:249:VAL:HG12	3:D:302:MET:HE3	2.00	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:247:GLU:O	3:C:302:MET:HE1	2.18	0.43
3:C:409:GLU:OE1	3:C:409:GLU:HA	2.17	0.43
3:D:364:GLN:HA	3:D:365:PRO:HD3	1.75	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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:C:249:VAL:HG12	3:C:302:MET:HE3	2.00	0.41
3:C:231:ASP:OD2	3:C:233:THR:OG1	2.33	0.41
3:D:294:VAL:HG22	3:D:295:GLY:N	2.35	0.41
3:D:393:ASN:O	3:D:395:LEU:HD22	2.19	0.41
3:D:381:VAL:CG1	3:D:435:TYR:HB3	2.42	0.41
3:C:315:ARG:O	3:C:318:ASP:HB2	2.20	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:237:PHE:CD2	3:C:307:ASP:HA	2.55	0.41
3:D:315:ARG:O	3:D:316:ASN:C	2.59	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
2:B:5004:DT:H2''	2:B:5005:DA:OP2	2.21	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:452:THR:HG23	3:D:455:GLY:N	2.35	0.41
1:A:4013:DT:OP2	3:D:222:THR:CG2	2.69	0.41
3:D:240:VAL:HG11	3:D:251:LEU:HD21	2.03	0.41
1:A:4011:DA:C1'	1:A:4012:DA:H5''	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:403:GLN:HG3	3:C:413:LYS:HG2	2.03	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
3:C:395:LEU:N	3:C:398:THR:CG2	2.85	0.40
1:A:4013:DT:P	3:D:222:THR:HG21	2.60	0.40
3:C:298:PRO:C	3:C:300:ASN:N	2.75	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%)	4	15
3	D	279/281 (99%)	247 (88%)	24 (9%)	8 (3%)	4	15
All	All	558/562 (99%)	487 (87%)	55 (10%)	16 (3%)	4	15

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

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Mol	Chain	Res	Type
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%)	236 (95%)	13 (5%)	23	51
3	D	249/249 (100%)	237 (95%)	12 (5%)	25	55
All	All	498/498 (100%)	473 (95%)	25 (5%)	24	53

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	188	LYS
3	C	189	LYS
3	C	225	SER
3	C	239	THR
3	C	246	ASN
3	C	289	THR
3	C	314	LEU
3	C	346	LYS
3	C	361	LEU
3	C	395	LEU
3	C	396	LYS
3	C	405	ASN
3	C	449	TYR
3	D	188	LYS
3	D	189	LYS
3	D	239	THR

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Mol	Chain	Res	Type
3	D	246	ASN
3	D	289	THR
3	D	314	LEU
3	D	346	LYS
3	D	361	LEU
3	D	395	LEU
3	D	396	LYS
3	D	405	ASN
3	D	449	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	196	GLN
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	377	HIS
3	D	393	ASN
3	D	405	ASN
3	D	426	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

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%)	-0.12	1 (6%) 17 13	28, 46, 72, 82	0
2	B	15/15 (100%)	-0.25	0 100 100	28, 44, 62, 74	0
3	C	281/281 (100%)	0.31	25 (8%) 9 6	28, 70, 104, 127	0
3	D	281/281 (100%)	0.38	14 (4%) 28 24	27, 72, 100, 122	0
All	All	592/592 (100%)	0.32	40 (6%) 17 13	27, 70, 103, 127	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	408	ASP	10.2
3	D	409	GLU	6.6
3	C	189	LYS	6.3
3	C	409	GLU	6.1
3	C	329	LYS	5.7
3	C	328	SER	5.4
3	D	276	ARG	4.4
3	D	189	LYS	4.1
3	C	348	GLY	3.9
3	C	325	ILE	3.9
3	D	295	GLY	3.5
3	C	458	HIS	3.0
3	D	188	LYS	3.0
3	C	442	LEU	3.0
3	C	326	ALA	3.0
3	C	323	ILE	3.0
3	C	408	ASP	3.0
3	C	438	GLN	2.9
3	C	327	GLY	2.9
3	C	248	PRO	2.9
3	C	330	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
3	C	324	GLY	2.7
3	C	440	ILE	2.7
3	D	346	LYS	2.7
3	D	438	GLN	2.6
3	C	247	GLU	2.6
3	C	346	LYS	2.6
3	D	368	VAL	2.5
3	C	322	ARG	2.4
3	D	217	ARG	2.3
3	C	321	ALA	2.3
3	C	347	ASP	2.3
3	D	439	HIS	2.2
3	D	410	ASN	2.2
3	D	382	LYS	2.1
3	D	344	MET	2.1
1	A	4001	DT	2.1
3	C	192	MET	2.1
3	C	456	ARG	2.0
3	C	443	PRO	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 carbohydrates 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.