Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:04 PM GMT

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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

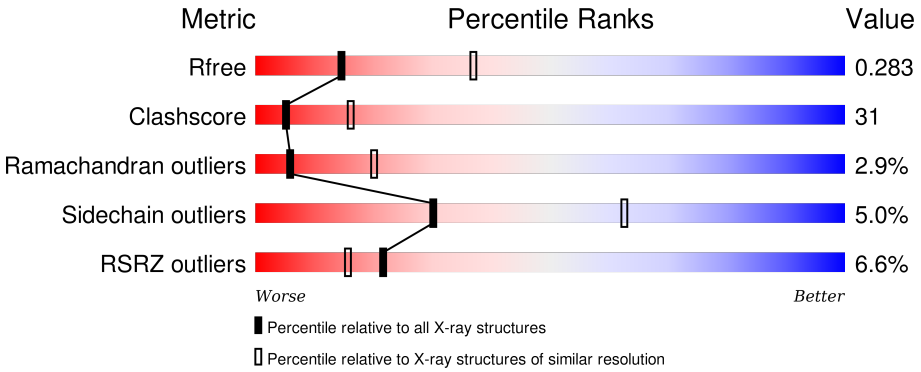
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	2228 (2.90-2.82)
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (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. 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 <=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	9% 54% 42% 5%
3	D	281	5% 53% 43% .

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.

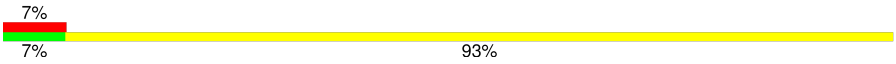
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	281	Total	C	N	O	S	0	0	0
			2184	1371	389	414	10			
3	D	281	Total	C	N	O	S	0	0	0
			2184	1371	389	414	10			

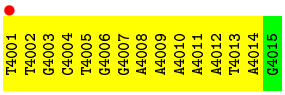
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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'

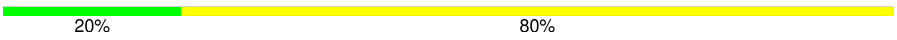
Chain A:

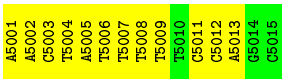




- Molecule 2: 5'-D(*AP*AP*CP*TP*AP*TP*TP*TP*TP*TP*CP*CP*AP*GP*C)-3'

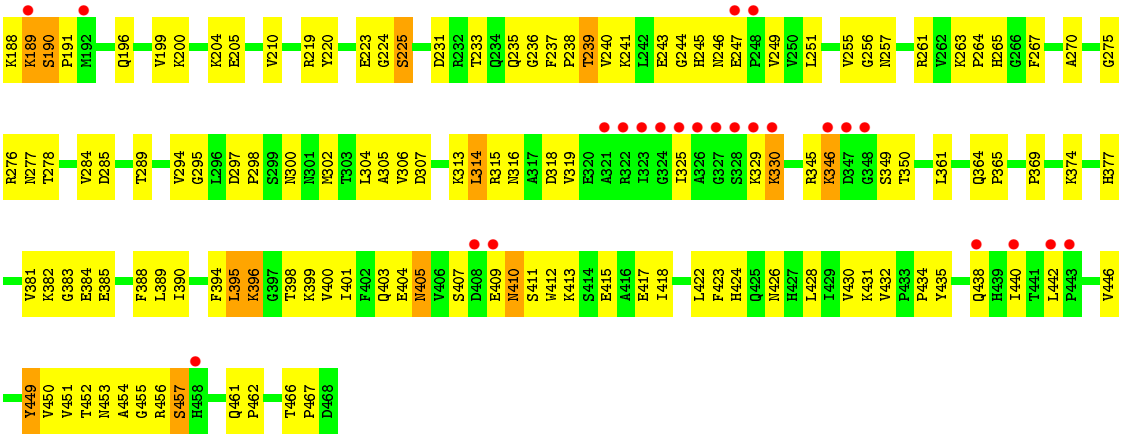
Chain B:





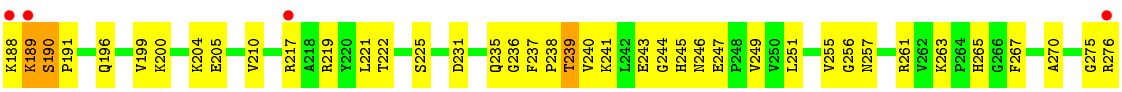
- Molecule 3: NUCLEAR FACTOR OF ACTIVATED T CELLS 5

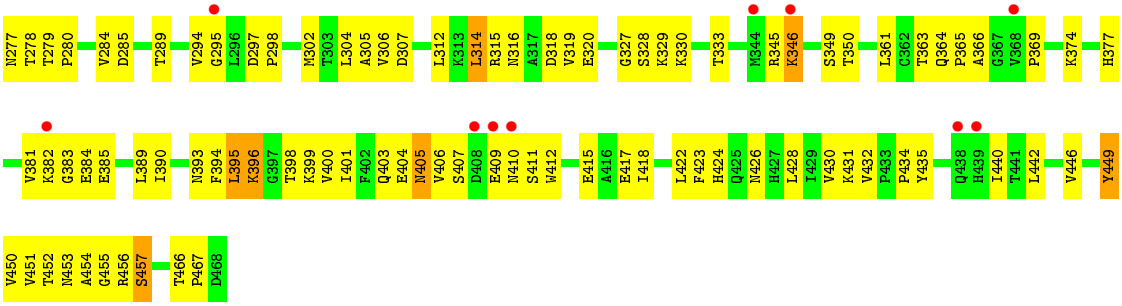
Chain C:



- Molecule 3: NUCLEAR FACTOR OF ACTIVATED T CELLS 5

Chain D:




N277 T278 T279 P280 V284 D285 T289 V294 G295 L296 D297 P298 M302 T303 L304 A305 V306 D307 L312 K313 L314 R315 N316 A317 D318 V319 E320 G327 S328 K329 K330 T333 M344 R345 K346 S349 T350 L361 C362 T363 Q364 P365 A366 G367 V368 P369 K374 H377
V381 K382 G383 E384 E385 L389 I390 N393 F394 L395 K396 G397 T398 K399 V400 I401 F402 Q403 E404 N405 V406 S407 D408 E409 N410 S411 W412 E415 A416 E417 I418 L422 F423 H424 Q425 N426 H427 L428 I429 V430 K431 V432 P433 P434 Y435 Q438 H439 I440 T441 L442 V446 Y449
V450 V451 T452 N453 A454 G455 R456 S457 T466 P467 D468

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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 (7.20%)	DCC
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
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Outliers	2 of 21103 reflections (0.009%)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.68	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

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:297:ASP:CG	3:C:298:PRO:HD2	2.12	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

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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:D:381:VAL:HG23	3:D:466:THR:O	1.96	0.63
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: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:452:THR:HG23	3:D:454:ALA:H	1.63	0.62
3:D:389:LEU:HD12	3:D:428:LEU:HD11	1.81	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:304:LEU:HD22	3:D:305:ALA:N	2.15	0.61
3:D:267:PHE:CE1	3:D:319:VAL:HG11	2.36	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
3:C:418:ILE:HG12	3:C:430:VAL:HG12	1.84	0.60
1:A:4011:DA:H2"	1:A:4012:DA:H5"	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:D:396:LYS:CE	3:D:396:LYS:HA	2.27	0.59
3:C:245:HIS:CD2	3:C:247:GLU:H	2.21	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:245:HIS:CD2	3:D:247:GLU:H	2.20	0.59
3:C:345:ARG:NH1	3:C:349:SER:HB2	2.18	0.59
3:D:278:THR:HA	3:D:307:ASP:OD2	2.02	0.58
3:C:256:GLY:HA2	3:C:265:HIS:H	1.68	0.58
3:C:385:GLU:O	3:C:432:VAL:HG23	2.04	0.58
3:D:418:ILE:HG12	3:D:430:VAL:HG12	1.83	0.58
2:B:5006:DT:H2"	2:B:5007:DT:H5'	1.85	0.58
3:D:239:THR:HG23	3:D:305:ALA:CA	2.34	0.58
3:C:245:HIS:HD2	3:C:247:GLU:H	1.52	0.58
3:D:210:VAL:O	3:D:238:PRO:HA	2.03	0.58
3:D:369:PRO:HD3	3:D:452:THR:HG21	1.86	0.57
1:A:4011:DA:C2'	1:A:4012:DA:H5"	2.34	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:D:221:LEU:N	3:D:312:LEU:HD11	2.19	0.57
3:C:382:LYS:O	3:C:434:PRO:HB3	2.05	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:D:221:LEU:HD23	3:D:221:LEU:C	2.25	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: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:452:THR:C	3:D:454:ALA:H	2.11	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:398:THR:HA	3:C:451:VAL:O	2.08	0.54
3:C:196:GLN:HE22	3:C:261:ARG:NH1	2.02	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
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:5001:DA:H8	2:B:5001:DA:O5'	1.91	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:D:346:LYS:CA	3:D:346:LYS:HE3	2.34	0.52
3:D:251:LEU:HB3	3:D:294:VAL:CG1	2.39	0.52
3:C:255:VAL:HG23	3:C:270:ALA:HB2	1.91	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:D:395:LEU:O	3:D:398:THR:HG23	2.09	0.51
3:C:346:LYS:HE3	3:C:346:LYS:CA	2.35	0.51
3:D:384:GLU:HA	3:D:384:GLU:OE1	2.10	0.51
3:D:284:VAL:HG22	3:D:285:ASP:N	2.25	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:D:452:THR:C	3:D:454:ALA:N	2.64	0.51
3:C:407:SER:CB	3:C:411:SER:HB3	2.34	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:422:LEU:HD13	3:D:390:ILE:HD11	1.93	0.50
3:C:284:VAL:HG22	3:C:285:ASP:N	2.26	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:D:261:ARG:HB3	3:D:261:ARG:NH1	2.27	0.49
3:C:440:ILE:HG13	3:C:467:PRO:HG3	1.94	0.49
3:D:395:LEU:HD23	3:D:452:THR:OG1	2.10	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
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:346:LYS:HA	3:D:346:LYS:CE	2.38	0.49
3:D:304:LEU:HD22	3:D:305:ALA:H	1.78	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:261:ARG:HB3	3:C:261:ARG:HH11	1.77	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: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:327:GLY:C	3:D:329:LYS:H	2.17	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:D:452:THR:HG23	3:D:455:GLY:H	1.78	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:C:369:PRO:HG2	3:C:457:SER:N	2.30	0.47
3:D:440:ILE:HG13	3:D:467:PRO:HG3	1.95	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:C:275:GLY:C	3:C:277:ASN:H	2.17	0.47
3:D:190:SER:N	3:D:191:PRO:CD	2.77	0.47
2:B:5001:DA:C8	2:B:5001:DA:O5'	2.65	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:219:ARG:NH1	3:C:223:GLU:O	2.49	0.45
3:C:190:SER:N	3:C:191:PRO:CD	2.79	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:D:316:ASN:O	3:D:320:GLU:HG3	2.18	0.44
3:D:199:VAL:HG13	3:D:200:LYS:N	2.32	0.44
3:C:417:GLU:OE1	3:C:431:LYS:HE2	2.17	0.44
3:C:364:GLN:HA	3:C:365:PRO:HD3	1.82	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: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:409:GLU:OE1	3:C:409:GLU:HA	2.17	0.43
3:C:247:GLU:O	3:C:302:MET:HE1	2.18	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:325:ILE:O	3:C:329:LYS:CB	2.67	0.43
3:C:294:VAL:HG22	3:C:295:GLY:N	2.34	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:315:ARG:CG	3:D:318:ASP:OD2	2.61	0.42
3:D:251:LEU:HD23	3:D:294:VAL:HG11	2.00	0.42
3:D:400:VAL:HA	3:D:450:VAL:HG12	2.00	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:267:PHE:O	3:D:314:LEU:HB2	2.19	0.42
3:D:237:PHE:CD2	3:D:307:ASP:HA	2.55	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:381:VAL:HG12	3:C:438:GLN:OE1	2.19	0.42
3:C:256:GLY:HA2	3:C:264:PRO:HA	2.02	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: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:240:VAL:HG11	3:C:251:LEU:HD21	2.01	0.41
3:C:249:VAL:HG12	3:C:302:MET:HE3	2.00	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:D:294:VAL:HG22	3:D:295:GLY:N	2.35	0.41
3:C:231:ASP:OD2	3:C:233:THR:OG1	2.33	0.41
3:D:279:THR:HG23	3:D:280:PRO:HD2	2.02	0.41
3:C:315:ARG:O	3:C:318:ASP:HB2	2.20	0.41
2:B:5006:DT:H2"	2:B:5007:DT:C5'	2.51	0.41
3:D:315:ARG:O	3:D:316:ASN:C	2.59	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
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
2:B:5004:DT:H2"	2:B:5005:DA:OP2	2.21	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
3:C:251:LEU:HD23	3:C:294:VAL:HG11	2.02	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:400:VAL:HG21	3:C:430:VAL:CG1	2.30	0.40
3:C:374:LYS:HA	3:C:388:PHE:O	2.21	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:399:LYS:HB2	3:C:451:VAL:HG23	2.02	0.40
3:C:298:PRO:C	3:C:300:ASN:N	2.75	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%)	6 20
3	D	279/281 (99%)	247 (88%)	24 (9%)	8 (3%)	6 20
All	All	558/562 (99%)	487 (87%)	55 (10%)	16 (3%)	6 20

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%)	29	60
3	D	249/249 (100%)	237 (95%)	12 (5%)	31	65
All	All	498/498 (100%)	473 (95%)	25 (5%)	30	62

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, 95^{th} 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%)	-0.06	1 (6%) 21 15	28, 46, 72, 82	0
2	B	15/15 (100%)	-0.20	0 100 100	28, 44, 62, 74	0
3	C	281/281 (100%)	0.32	24 (8%) 13 8	28, 70, 104, 127	0
3	D	281/281 (100%)	0.40	14 (4%) 32 26	27, 72, 100, 122	0
All	All	592/592 (100%)	0.34	39 (6%) 22 16	27, 70, 103, 127	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	408	ASP	10.5
3	D	409	GLU	6.8
3	C	189	LYS	6.4
3	C	409	GLU	6.2
3	C	329	LYS	5.8
3	C	328	SER	5.6
3	D	276	ARG	4.2
3	D	189	LYS	4.2
3	C	325	ILE	4.0
3	C	348	GLY	4.0
3	D	295	GLY	3.6
3	C	458	HIS	3.1
3	D	188	LYS	3.1
3	C	408	ASP	3.1
3	C	438	GLN	3.1
3	C	442	LEU	3.0
3	C	248	PRO	3.0
3	C	323	ILE	2.9
3	C	326	ALA	2.9
3	C	330	LYS	2.9
3	C	327	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
3	C	324	GLY	2.8
3	D	346	LYS	2.8
3	C	440	ILE	2.7
3	D	438	GLN	2.7
3	C	247	GLU	2.6
3	C	346	LYS	2.6
3	D	368	VAL	2.5
3	C	347	ASP	2.4
3	C	322	ARG	2.3
1	A	4001	DT	2.3
3	D	410	ASN	2.3
3	D	439	HIS	2.3
3	D	217	ARG	2.3
3	C	321	ALA	2.2
3	D	382	LYS	2.2
3	D	344	MET	2.1
3	C	192	MET	2.1
3	C	443	PRO	2.1

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.