



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 16, 2026 – 10:20 AM UTC

PDB ID : 2I9T / pdb_00002i9t
Title : Structure of NF-kB p65-p50 heterodimer bound to PRDII element of B-interferon promoter
Authors : Escalante, C.R.; Shen, L.; Thanos, D.; Aggarwal, A.K.
Deposited on : 2006-09-06
Resolution : 2.80 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

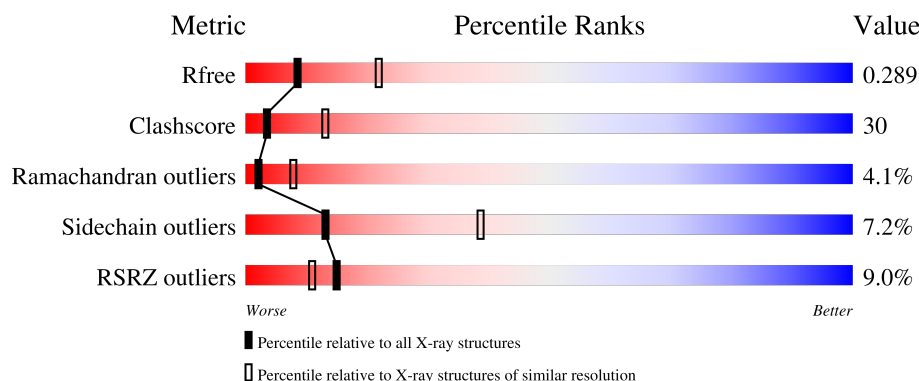
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	C	17	6% 6% 76% 18%
2	D	17	12% 18% 82%
3	A	279	6% 60% 32% 5% ..
4	B	313	11% 51% 40% 8%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5226 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(*AP*GP*TP*GP*GP*GP*AP*AP*AP*TP*TP*C P*CP*TP*CP*TP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	17	Total	C	N	O	P	0	0	0
			348	167	64	101	16			

- Molecule 2 is a DNA chain called 5'-D(*CP*AP*GP*AP*GP*GP*AP*AP*TP*TP*TP*C P*CP*CP*AP*CP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	17	Total	C	N	O	P	0	0	0
			343	165	63	99	16			

- Molecule 3 is a protein called Transcription factor p65.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	275	Total	C	N	O	S	0	0	0
			2122	1324	393	394	11			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	GLY	-	cloning artifact	UNP Q04207
A	14	SER	-	cloning artifact	UNP Q04207
A	15	HIS	-	cloning artifact	UNP Q04207
A	16	MET	-	cloning artifact	UNP Q04207
A	17	HIS	-	cloning artifact	UNP Q04207
A	18	ALA	-	cloning artifact	UNP Q04207

- Molecule 4 is a protein called Nuclear factor NF-kappa-B p105 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	312	Total	C	N	O	S	0	0	0
			2392	1517	423	440	12			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	338	MET	-	initiating methionine	UNP P25799

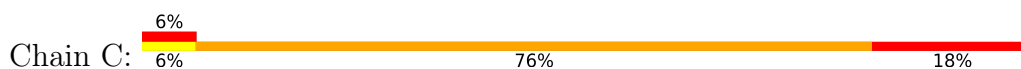
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	21	Total	O	0	0
			21	21		

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.

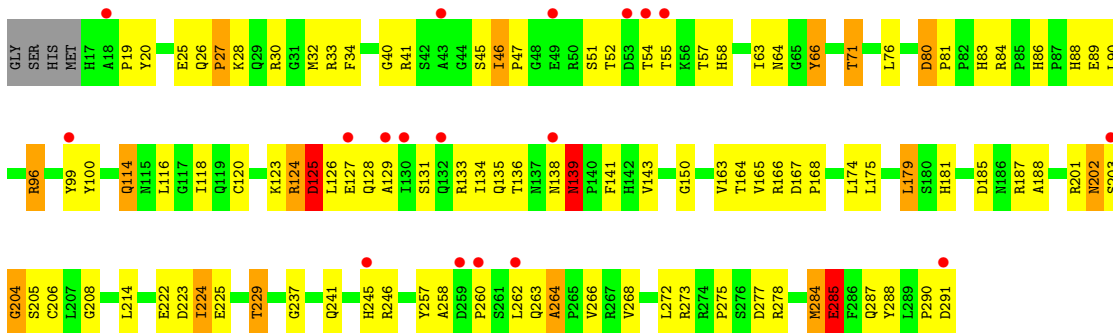
- Molecule 1: 5'-D(*AP*GP*TP*GP*GP*GP*AP*AP*AP*TP*TP*CP*CP*TP*CP*TP*G)-3',



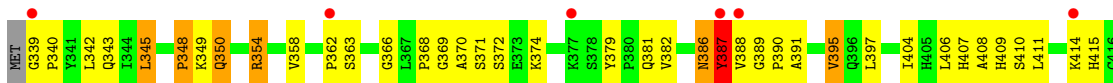
- Molecule 2: 5'-D(*CP*AP*GP*AP*GP*GP*AP*AP*TP*TP*TP*CP*CP*CP*AP*CP*T)-3',

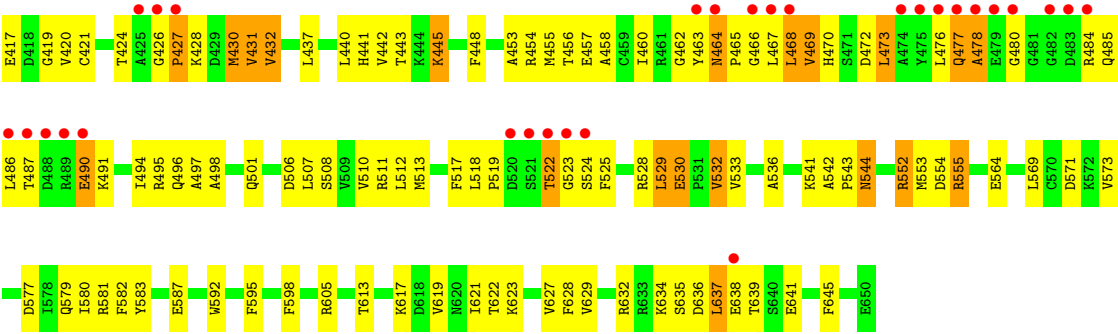


- Molecule 3: Transcription factor p65



- Molecule 4: Nuclear factor NF-kappa-B p105 subunit





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	97.62Å 166.11Å 60.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.46 – 2.80 34.46 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.3 (34.46-2.80) 99.3 (34.46-2.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.27 (at 2.81Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.233 , 0.288 0.237 , 0.289	Depositor DCC
R_{free} test set	2438 reflections (9.89%)	wwPDB-VP
Wilson B-factor (Å ²)	59.0	Xtriage
Anisotropy	0.256	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 63.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5226	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.52% 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	C	0.36	0/390	1.61	18/601 (3.0%)
2	D	0.35	0/384	0.81	0/590
3	A	0.49	0/2176	0.99	8/2958 (0.3%)
4	B	0.46	0/2444	0.97	11/3304 (0.3%)
All	All	0.46	0/5394	1.03	37/7453 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	5

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	428	LYS	N-CA-C	-9.32	101.60	113.16
4	B	529	LEU	N-CA-C	7.28	121.02	112.72
1	C	705	DG	C2'-C3'-O3'	-7.21	100.69	111.50
1	C	704	DG	C2'-C3'-O3'	-6.95	101.08	111.50
1	C	706	DG	C2'-C3'-O3'	-6.87	101.19	111.50
1	C	710	DT	C2'-C3'-O3'	-6.86	101.21	111.50
1	C	710	DT	N1-C1'-C2'	6.83	123.75	113.50
1	C	701	DA	C2'-C3'-O3'	-6.69	101.46	111.50
1	C	712	DC	C2'-C3'-O3'	-6.53	101.71	111.50
3	A	80	ASP	CA-C-N	6.45	124.31	119.66
3	A	80	ASP	C-N-CA	6.45	124.31	119.66
4	B	530	GLU	CA-C-N	6.41	126.78	119.92
4	B	530	GLU	C-N-CA	6.41	126.78	119.92
4	B	386	ASN	N-CA-C	-6.36	102.62	111.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	709	DA	C2'-C3'-O3'	-6.33	102.01	111.50
1	C	708	DA	C2'-C3'-O3'	-6.25	102.12	111.50
1	C	712	DC	N1-C1'-C2'	6.25	122.87	113.50
1	C	702	DG	C2'-C3'-O3'	-6.20	102.20	111.50
1	C	707	DA	C2'-C3'-O3'	-6.10	102.35	111.50
1	C	703	DT	C2'-C3'-O3'	-6.08	102.37	111.50
1	C	711	DT	N1-C1'-C2'	6.06	122.59	113.50
4	B	348	PRO	N-CA-C	-6.05	102.33	111.41
1	C	709	DA	N9-C1'-C2'	5.84	122.26	113.50
4	B	637	LEU	N-CA-C	-5.77	105.82	112.86
4	B	635	SER	N-CA-C	5.66	117.14	110.97
3	A	188	ALA	CA-C-N	5.65	125.77	119.32
3	A	188	ALA	C-N-CA	5.65	125.77	119.32
1	C	713	DC	N1-C1'-C2'	5.64	121.96	113.50
3	A	27	PRO	N-CA-C	-5.55	102.40	111.68
1	C	711	DT	C2'-C3'-O3'	-5.50	103.25	111.50
1	C	716	DT	C2'-C3'-O3'	-5.38	103.42	111.50
3	A	20	TYR	N-CA-C	5.26	117.19	109.24
3	A	40	GLY	N-CA-C	5.26	118.70	112.33
4	B	431	VAL	N-CA-C	5.23	114.28	106.85
4	B	473	LEU	N-CA-C	-5.22	106.77	112.72
3	A	237	GLY	N-CA-C	-5.08	105.59	112.14
4	B	464	ASN	N-CA-C	5.03	120.93	109.81

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	702	DG	Sidechain
1	C	703	DT	Sidechain
1	C	709	DA	Sidechain
1	C	714	DT	Sidechain
1	C	715	DC	Sidechain

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	C	348	0	194	27	0
2	D	343	0	193	31	0
3	A	2122	0	2011	103	0
4	B	2392	0	2344	142	0
5	B	21	0	0	0	3
All	All	5226	0	4742	294	3

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 30.

All (294) 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)
4:B:470:HIS:HB3	4:B:473:LEU:HB2	1.30	1.08
2:D:721:DA:H2''	2:D:722:DG:H5''	1.39	1.04
2:D:732:DA:H2''	2:D:733:DC:H5''	1.43	0.98
4:B:342:LEU:HD12	4:B:532:VAL:HG11	1.47	0.96
2:D:732:DA:C2'	2:D:733:DC:H5''	1.96	0.95
3:A:224:ILE:HD13	3:A:225:GLU:H	1.33	0.93
4:B:388:VAL:HG21	4:B:518:LEU:HD22	1.53	0.90
3:A:284:MET:O	3:A:285:GLU:HB3	1.72	0.89
4:B:388:VAL:CG2	4:B:518:LEU:HD22	2.04	0.87
4:B:388:VAL:HG11	4:B:518:LEU:HD13	1.59	0.85
4:B:349:LYS:O	4:B:350:GLN:HB2	1.79	0.82
3:A:33:ARG:HH21	3:A:187:ARG:HH21	1.27	0.82
4:B:627:VAL:HG12	4:B:628:PHE:H	1.44	0.81
2:D:721:DA:C2'	2:D:722:DG:H5''	2.11	0.81
3:A:33:ARG:NH2	3:A:187:ARG:HH21	1.80	0.80
2:D:729:DC:H2''	2:D:730:DC:H5'	1.63	0.80
4:B:627:VAL:HG12	4:B:628:PHE:N	1.98	0.79
4:B:390:PRO:HA	4:B:426:GLY:HA2	1.63	0.78
4:B:388:VAL:HG21	4:B:518:LEU:HD13	1.65	0.77
4:B:622:THR:HG22	4:B:623:LYS:HD3	1.65	0.77
3:A:99:TYR:OH	3:A:133:ARG:HD3	1.85	0.75
1:C:710:DT:H2''	1:C:711:DT:O5'	1.86	0.75
3:A:71:THR:HG23	3:A:164:THR:HB	1.67	0.75
2:D:732:DA:C3'	2:D:733:DC:H5''	2.16	0.75
4:B:470:HIS:HB3	4:B:473:LEU:CB	2.13	0.75
3:A:167:ASP:HB2	3:A:168:PRO:HD2	1.66	0.75
3:A:205:SER:HB2	3:A:291:ASP:OXT	1.85	0.74
3:A:19:PRO:HG2	3:A:175:LEU:HD11	1.68	0.73
3:A:245:HIS:ND1	4:B:569:LEU:HD13	2.03	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:224:ILE:HD13	3:A:225:GLU:N	2.03	0.72
4:B:522:THR:HG22	4:B:523:GLY:H	1.53	0.72
3:A:28:LYS:HD2	3:A:30:ARG:O	1.89	0.72
4:B:445:LYS:H	4:B:445:LYS:HD3	1.55	0.72
1:C:704:DG:H2''	1:C:705:DG:O5'	1.91	0.70
2:D:723:DG:H1'	2:D:724:DA:H5''	1.73	0.69
4:B:407:HIS:CD2	4:B:510:VAL:HG12	2.28	0.69
3:A:26:GLN:HE21	3:A:27:PRO:HD2	1.57	0.69
4:B:544:ASN:HD22	4:B:544:ASN:C	2.00	0.69
4:B:522:THR:HG22	4:B:523:GLY:N	2.08	0.68
3:A:33:ARG:HH21	3:A:187:ARG:NH2	1.92	0.68
3:A:139:ASN:HD21	3:A:143:VAL:HG22	1.58	0.68
3:A:263:GLN:HA	3:A:290:PRO:HB3	1.75	0.68
4:B:345:LEU:HD23	4:B:381:GLN:OE1	1.94	0.68
4:B:388:VAL:HG23	4:B:388:VAL:O	1.92	0.68
4:B:445:LYS:H	4:B:445:LYS:CD	2.06	0.68
4:B:448:PHE:HE1	4:B:495:ARG:HH11	1.39	0.67
4:B:395:VAL:HG13	4:B:421:CYS:HB3	1.74	0.67
2:D:726:DT:H2''	2:D:727:DT:H5'	1.76	0.67
3:A:165:VAL:HG22	3:A:175:LEU:HD21	1.76	0.67
4:B:388:VAL:HG21	4:B:518:LEU:CD2	2.24	0.67
3:A:66:TYR:CE2	3:A:165:VAL:HB	2.30	0.67
4:B:342:LEU:HD12	4:B:532:VAL:CG1	2.23	0.67
4:B:350:GLN:HG3	4:B:536:ALA:O	1.94	0.66
2:D:728:DT:H2''	2:D:729:DC:C5'	2.26	0.66
3:A:245:HIS:CG	4:B:569:LEU:HD13	2.31	0.66
3:A:28:LYS:HE3	3:A:32:MET:H	1.60	0.66
4:B:627:VAL:CG1	4:B:628:PHE:H	2.08	0.65
1:C:714:DT:H2'	1:C:715:DC:C6	2.31	0.65
4:B:579:GLN:NE2	4:B:632:ARG:HE	1.94	0.65
4:B:349:LYS:O	4:B:350:GLN:CB	2.45	0.65
4:B:387:TYR:HB2	4:B:430:MET:HG2	1.77	0.65
2:D:719:DA:H1'	2:D:720:DG:H5'	1.80	0.64
3:A:99:TYR:HE1	3:A:136:THR:HG21	1.62	0.64
1:C:704:DG:H2''	1:C:705:DG:C5'	2.28	0.64
3:A:28:LYS:HG2	3:A:47:PRO:HG2	1.80	0.64
4:B:342:LEU:HD13	4:B:343:GLN:N	2.12	0.64
3:A:245:HIS:CE1	4:B:569:LEU:CD1	2.81	0.63
4:B:464:ASN:C	4:B:466:GLY:H	2.07	0.63
4:B:426:GLY:H	4:B:427:PRO:HD3	1.63	0.63
3:A:52:THR:CG2	3:A:55:THR:H	2.13	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:727:DT:H1'	2:D:728:DT:H5''	1.81	0.61
2:D:732:DA:H2''	2:D:733:DC:C5'	2.24	0.61
3:A:96:ARG:HG3	3:A:96:ARG:HH11	1.63	0.61
4:B:511:ARG:HG2	4:B:536:ALA:HA	1.83	0.61
1:C:712:DC:H2''	1:C:713:DC:O5'	2.00	0.60
4:B:592:TRP:CD1	4:B:617:LYS:HG3	2.35	0.60
3:A:166:ARG:HG2	3:A:166:ARG:HH11	1.67	0.60
3:A:245:HIS:ND1	4:B:569:LEU:CD1	2.64	0.60
4:B:391:ALA:O	4:B:424:THR:HG23	2.01	0.60
3:A:45:SER:HA	3:A:116:LEU:O	2.01	0.60
4:B:627:VAL:CG1	4:B:628:PHE:N	2.65	0.60
4:B:349:LYS:HB2	4:B:368:PRO:HG2	1.82	0.60
3:A:52:THR:HG22	3:A:55:THR:OG1	2.02	0.59
3:A:28:LYS:O	3:A:28:LYS:HG3	2.03	0.59
4:B:426:GLY:N	4:B:427:PRO:HD3	2.18	0.59
1:C:716:DT:H2'	1:C:717:DG:C8	2.38	0.59
4:B:354:ARG:HD3	4:B:541:LYS:HG3	1.85	0.59
4:B:552:ARG:HG3	4:B:553:MET:N	2.17	0.58
3:A:81:PRO:HG3	3:A:83:HIS:NE2	2.18	0.58
4:B:388:VAL:HG21	4:B:518:LEU:CD1	2.32	0.58
4:B:339:GLY:O	4:B:386:ASN:ND2	2.35	0.58
1:C:703:DT:OP2	4:B:363:SER:HA	2.03	0.58
4:B:404:ILE:O	4:B:467:LEU:HG	2.03	0.58
3:A:125:ASP:OD2	3:A:125:ASP:N	2.37	0.58
3:A:222:GLU:HA	3:A:241:GLN:NE2	2.18	0.58
3:A:263:GLN:O	3:A:264:ALA:HB3	2.03	0.58
4:B:496:GLN:HE21	4:B:496:GLN:HA	1.69	0.58
1:C:710:DT:P	3:A:123:LYS:HG2	2.44	0.57
3:A:27:PRO:HB2	3:A:46:ILE:HD11	1.86	0.57
3:A:34:PHE:CD2	3:A:185:ASP:HB2	2.40	0.57
4:B:484:ARG:HD2	4:B:485:GLN:O	2.04	0.57
1:C:701:DA:H2'	1:C:702:DG:C8	2.39	0.57
1:C:709:DA:H2''	1:C:710:DT:O5'	2.05	0.57
3:A:89:GLU:HG2	3:A:133:ARG:NH2	2.20	0.56
2:D:728:DT:H2''	2:D:729:DC:H5''	1.88	0.56
4:B:388:VAL:CG1	4:B:518:LEU:HD13	2.31	0.56
4:B:519:PRO:HA	4:B:524:SER:O	2.05	0.56
4:B:564:GLU:O	4:B:613:THR:HG23	2.05	0.56
2:D:726:DT:H2''	2:D:727:DT:C5'	2.35	0.56
4:B:414:LYS:O	4:B:415:HIS:HB2	2.04	0.56
4:B:484:ARG:HD2	4:B:484:ARG:C	2.31	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:707:DA:H2'	1:C:708:DA:C8	2.41	0.56
4:B:426:GLY:N	4:B:427:PRO:CD	2.69	0.56
3:A:257:TYR:CG	3:A:258:ALA:N	2.74	0.56
4:B:387:TYR:HB2	4:B:430:MET:CG	2.35	0.56
4:B:387:TYR:CB	4:B:430:MET:HG2	2.35	0.56
3:A:26:GLN:NE2	3:A:181:HIS:H	2.04	0.55
4:B:518:LEU:HD11	4:B:529:LEU:HD11	1.86	0.55
3:A:229:THR:O	3:A:268:VAL:HB	2.06	0.55
4:B:340:PRO:HB2	4:B:529:LEU:HD21	1.89	0.55
4:B:480:GLY:O	4:B:484:ARG:HB3	2.07	0.55
4:B:629:VAL:HG23	4:B:645:PHE:HB2	1.89	0.55
4:B:580:ILE:HD12	4:B:580:ILE:N	2.21	0.54
4:B:579:GLN:HE21	4:B:632:ARG:HE	1.55	0.54
4:B:583:TYR:O	4:B:627:VAL:HG13	2.06	0.54
3:A:34:PHE:CE2	3:A:185:ASP:HB2	2.43	0.54
4:B:513:MET:HE2	4:B:533:VAL:HG22	1.90	0.54
1:C:702:DG:H3'	4:B:363:SER:HB2	1.90	0.54
2:D:732:DA:H2''	2:D:733:DC:O4'	2.07	0.54
1:C:715:DC:H2'	1:C:716:DT:C6	2.43	0.54
4:B:544:ASN:C	4:B:544:ASN:ND2	2.62	0.53
2:D:728:DT:H5'	2:D:728:DT:H6	1.74	0.53
3:A:203:SER:O	3:A:287:GLN:O	2.25	0.53
2:D:728:DT:H1'	2:D:729:DC:H5''	1.90	0.53
4:B:571:ASP:O	4:B:573:VAL:HG13	2.08	0.53
3:A:51:SER:HB2	3:A:57:THR:OG1	2.09	0.53
1:C:711:DT:H2''	1:C:712:DC:O5'	2.07	0.53
4:B:388:VAL:CG2	4:B:518:LEU:HD13	2.36	0.53
2:D:728:DT:C2'	2:D:729:DC:H5''	2.39	0.52
4:B:448:PHE:HE1	4:B:495:ARG:NH1	2.04	0.52
4:B:348:PRO:HG3	4:B:512:LEU:HD12	1.91	0.52
2:D:728:DT:H2''	2:D:729:DC:H5'	1.90	0.52
3:A:245:HIS:CE1	4:B:569:LEU:HD12	2.44	0.52
3:A:258:ALA:O	3:A:260:PRO:HD3	2.10	0.52
3:A:27:PRO:CB	3:A:46:ILE:HD11	2.40	0.52
2:D:721:DA:C3'	2:D:722:DG:H5''	2.38	0.52
3:A:202:ASN:C	3:A:202:ASN:HD22	2.18	0.52
3:A:223:ASP:OD2	3:A:275:PRO:HD2	2.10	0.51
4:B:466:GLY:O	4:B:467:LEU:HB3	2.11	0.51
4:B:490:GLU:O	4:B:494:ILE:N	2.42	0.51
4:B:506:ASP:C	4:B:508:SER:H	2.19	0.51
4:B:395:VAL:CG1	4:B:421:CYS:HB3	2.41	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:214:LEU:C	3:A:214:LEU:HD23	2.36	0.50
4:B:388:VAL:HG21	4:B:518:LEU:CG	2.41	0.50
4:B:442:VAL:HG22	4:B:443:THR:N	2.26	0.50
4:B:519:PRO:HG3	4:B:525:PHE:CE1	2.46	0.50
4:B:579:GLN:HE22	4:B:632:ARG:HH21	1.59	0.50
1:C:702:DG:H2''	1:C:703:DT:O5'	2.11	0.50
3:A:96:ARG:HG3	3:A:96:ARG:NH1	2.26	0.50
3:A:124:ARG:HG2	3:A:125:ASP:OD2	2.11	0.50
4:B:464:ASN:C	4:B:466:GLY:N	2.70	0.50
3:A:277:ASP:O	3:A:278:ARG:HB2	2.12	0.50
3:A:46:ILE:HD12	3:A:47:PRO:N	2.27	0.49
2:D:718:DC:H2''	2:D:719:DA:C8	2.47	0.49
3:A:126:LEU:HD23	3:A:126:LEU:C	2.37	0.49
2:D:723:DG:H2''	2:D:724:DA:H5'	1.95	0.49
2:D:726:DT:H1'	2:D:727:DT:H5''	1.94	0.49
3:A:127:GLU:HG3	3:A:128:GLN:N	2.27	0.49
4:B:587:GLU:CD	4:B:587:GLU:N	2.71	0.49
1:C:709:DA:H2''	1:C:710:DT:C5'	2.42	0.49
4:B:580:ILE:HD13	4:B:598:PHE:CE2	2.47	0.49
2:D:723:DG:H2''	2:D:724:DA:C5'	2.43	0.49
3:A:202:ASN:HD22	3:A:202:ASN:H	1.61	0.49
3:A:203:SER:O	3:A:204:GLY:O	2.30	0.49
4:B:455:MET:SD	4:B:498:ALA:HB2	2.53	0.49
3:A:25:GLU:HA	3:A:25:GLU:OE2	2.12	0.48
3:A:201:ARG:HG3	3:A:202:ASN:N	2.28	0.48
3:A:32:MET:CE	3:A:118:ILE:HD12	2.43	0.48
3:A:114:GLN:OE1	3:A:114:GLN:N	2.39	0.48
3:A:175:LEU:N	3:A:175:LEU:HD22	2.29	0.48
3:A:175:LEU:HD22	3:A:175:LEU:H	1.78	0.48
4:B:496:GLN:HA	4:B:496:GLN:NE2	2.28	0.48
4:B:414:LYS:O	4:B:415:HIS:CB	2.62	0.48
3:A:133:ARG:O	3:A:136:THR:HG22	2.13	0.48
4:B:369:GLY:N	4:B:379:TYR:HA	2.27	0.48
1:C:706:DG:H2''	1:C:707:DA:O5'	2.14	0.48
3:A:46:ILE:HD12	3:A:46:ILE:C	2.39	0.48
3:A:52:THR:HG23	3:A:54:THR:H	1.79	0.48
2:D:723:DG:C1'	2:D:724:DA:H5''	2.42	0.47
3:A:52:THR:HG23	3:A:54:THR:N	2.29	0.47
2:D:727:DT:H2''	2:D:728:DT:H5'	1.96	0.47
3:A:174:LEU:HD23	3:A:174:LEU:H	1.79	0.47
4:B:477:GLN:O	4:B:478:ALA:HB2	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:63:ILE:O	3:A:64:ASN:C	2.58	0.47
4:B:522:THR:CG2	4:B:523:GLY:N	2.77	0.47
3:A:32:MET:HE1	3:A:118:ILE:HD12	1.96	0.47
3:A:263:GLN:O	3:A:264:ALA:CB	2.63	0.47
4:B:464:ASN:N	4:B:465:PRO:HD3	2.30	0.47
4:B:522:THR:CG2	4:B:523:GLY:H	2.24	0.47
3:A:224:ILE:HD11	3:A:272:LEU:HD22	1.97	0.46
3:A:163:VAL:HG12	3:A:164:THR:N	2.30	0.46
3:A:124:ARG:O	3:A:126:LEU:N	2.43	0.46
2:D:726:DT:H2'	2:D:727:DT:H71	1.96	0.46
3:A:266:VAL:O	3:A:266:VAL:HG13	2.16	0.46
1:C:705:DG:H2''	1:C:706:DG:O5'	2.16	0.46
3:A:202:ASN:C	3:A:202:ASN:ND2	2.72	0.46
4:B:579:GLN:HE21	4:B:632:ARG:NE	2.13	0.46
3:A:19:PRO:O	3:A:175:LEU:HD12	2.16	0.45
3:A:126:LEU:O	3:A:129:ALA:HB3	2.15	0.45
4:B:455:MET:HE1	4:B:501:GLN:OE1	2.17	0.45
3:A:138:ASN:O	3:A:139:ASN:C	2.59	0.45
1:C:713:DC:H2''	1:C:714:DT:C5'	2.47	0.45
3:A:206:CYS:HA	3:A:288:TYR:CD1	2.52	0.45
3:A:224:ILE:CD1	3:A:225:GLU:N	2.77	0.45
3:A:225:GLU:HG3	3:A:273:ARG:HB3	1.98	0.45
4:B:406:LEU:CD2	4:B:468:LEU:HD13	2.47	0.45
4:B:382:VAL:HG22	4:B:432:VAL:HG13	1.99	0.45
4:B:582:PHE:CD2	4:B:629:VAL:HG22	2.52	0.45
3:A:202:ASN:HD22	3:A:202:ASN:N	2.15	0.44
3:A:206:CYS:HA	3:A:288:TYR:HD1	1.83	0.44
1:C:704:DG:H2''	1:C:705:DG:H5'	1.99	0.44
4:B:349:LYS:HA	4:B:370:ALA:HA	1.98	0.44
4:B:517:PHE:C	4:B:518:LEU:HD23	2.43	0.44
4:B:388:VAL:HG11	4:B:518:LEU:CD1	2.39	0.44
4:B:410:SER:HB3	4:B:419:GLY:HA2	2.00	0.44
4:B:441:HIS:HD2	4:B:442:VAL:O	1.99	0.44
4:B:581:ARG:HD2	4:B:595:PHE:CE1	2.52	0.44
4:B:621:ILE:HD12	4:B:623:LYS:O	2.17	0.44
3:A:88:HIS:ND1	3:A:120:CYS:HA	2.31	0.44
4:B:366:GLY:HA2	4:B:437:LEU:O	2.18	0.44
4:B:389:GLY:O	4:B:430:MET:HE1	2.18	0.44
4:B:554:ASP:OD2	4:B:555:ARG:N	2.51	0.44
4:B:605:ARG:HG3	4:B:605:ARG:HH11	1.83	0.44
3:A:26:GLN:HE22	3:A:181:HIS:H	1.63	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:41:ARG:HA	3:A:41:ARG:NE	2.32	0.44
4:B:387:TYR:CE2	4:B:389:GLY:N	2.86	0.44
4:B:513:MET:CE	4:B:533:VAL:HG22	2.48	0.44
4:B:632:ARG:CG	4:B:639:THR:HG22	2.48	0.44
3:A:166:ARG:HG2	3:A:166:ARG:NH1	2.30	0.43
3:A:100:TYR:CD1	3:A:100:TYR:C	2.97	0.43
1:C:713:DC:H2''	1:C:714:DT:O5'	2.17	0.43
2:D:727:DT:H2''	2:D:728:DT:C5'	2.49	0.43
3:A:86:HIS:CE1	3:A:88:HIS:CD2	3.06	0.43
3:A:126:LEU:HD23	3:A:126:LEU:O	2.18	0.43
3:A:141:PHE:HE2	3:A:179:LEU:HD11	1.83	0.43
4:B:397:LEU:HG	4:B:411:LEU:HG	2.01	0.43
3:A:66:TYR:CZ	3:A:165:VAL:HB	2.53	0.43
4:B:340:PRO:HB2	4:B:529:LEU:CD2	2.48	0.43
1:C:709:DA:C2'	1:C:710:DT:O5'	2.67	0.43
4:B:456:THR:C	4:B:458:ALA:N	2.76	0.43
4:B:496:GLN:HE21	4:B:496:GLN:CA	2.28	0.43
3:A:139:ASN:ND2	3:A:143:VAL:HG22	2.31	0.43
2:D:729:DC:H2''	2:D:730:DC:C5'	2.43	0.42
4:B:390:PRO:O	4:B:525:PHE:HE1	2.02	0.42
4:B:455:MET:HE2	4:B:469:VAL:HG22	1.99	0.42
4:B:478:ALA:C	4:B:480:GLY:H	2.27	0.42
3:A:143:VAL:O	3:A:143:VAL:HG23	2.19	0.42
1:C:706:DG:H2''	1:C:707:DA:C5'	2.49	0.42
1:C:711:DT:H2''	1:C:712:DC:C5'	2.50	0.42
3:A:128:GLN:O	3:A:131:SER:HB2	2.19	0.42
4:B:632:ARG:CB	4:B:639:THR:HG22	2.50	0.42
2:D:723:DG:O6	3:A:33:ARG:NH2	2.49	0.42
3:A:76:LEU:HG	3:A:90:LEU:HG	2.02	0.42
3:A:80:ASP:HA	3:A:81:PRO:HD3	1.86	0.42
3:A:99:TYR:CE1	3:A:136:THR:HG21	2.48	0.42
4:B:463:TYR:C	4:B:465:PRO:HD3	2.44	0.42
4:B:387:TYR:HE2	4:B:389:GLY:HA2	1.84	0.42
4:B:407:HIS:ND1	4:B:408:ALA:N	2.68	0.42
4:B:453:ALA:O	4:B:457:GLU:HG3	2.20	0.42
1:C:708:DA:H2''	1:C:709:DA:O5'	2.20	0.42
4:B:513:MET:HE2	4:B:533:VAL:CG2	2.50	0.42
4:B:354:ARG:CD	4:B:541:LYS:HG3	2.49	0.41
4:B:629:VAL:CG2	4:B:645:PHE:HB2	2.50	0.41
1:C:707:DA:H2'	1:C:708:DA:H8	1.85	0.41
4:B:409:HIS:HB3	4:B:440:LEU:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:371:SER:O	4:B:372:SER:C	2.63	0.41
4:B:487:THR:O	4:B:491:LYS:HG3	2.21	0.41
4:B:454:ARG:HH11	4:B:454:ARG:HG2	1.85	0.41
4:B:486:LEU:HB2	4:B:491:LYS:HE3	2.03	0.41
4:B:542:ALA:HA	4:B:543:PRO:HD3	1.93	0.41
4:B:517:PHE:CE1	4:B:528:ARG:HG3	2.56	0.41
4:B:494:ILE:O	4:B:497:ALA:HB3	2.21	0.41
2:D:728:DT:C1'	2:D:729:DC:H5''	2.51	0.41
4:B:636:ASP:C	4:B:638:GLU:N	2.78	0.41
4:B:406:LEU:HD13	4:B:454:ARG:HG3	2.03	0.40
4:B:445:LYS:CD	4:B:445:LYS:N	2.80	0.40
4:B:577:ASP:OD1	4:B:634:LYS:HB2	2.21	0.40
4:B:460:ILE:C	4:B:462:GLY:N	2.78	0.40
4:B:431:VAL:O	4:B:431:VAL:HG12	2.22	0.40
4:B:390:PRO:CA	4:B:426:GLY:HA2	2.44	0.40
4:B:442:VAL:HG22	4:B:443:THR:H	1.84	0.40
1:C:714:DT:H2''	1:C:715:DC:O4'	2.21	0.40
3:A:58:HIS:CE1	3:A:114:GLN:HB3	2.56	0.40
3:A:266:VAL:HG13	3:A:288:TYR:HB2	2.03	0.40

All (3) 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)
5:B:808:HOH:O	5:B:822:HOH:O[2_555]	0.58	1.62
5:B:810:HOH:O	5:B:815:HOH:O[2_555]	1.53	0.67
5:B:816:HOH:O	5:B:826:HOH:O[2_555]	1.98	0.22

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	A	273/279 (98%)	232 (85%)	29 (11%)	12 (4%)	2	7
4	B	310/313 (99%)	261 (84%)	37 (12%)	12 (4%)	2	8
All	All	583/592 (98%)	493 (85%)	66 (11%)	24 (4%)	2	8

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	125	ASP
4	B	374	LYS
4	B	387	TYR
4	B	478	ALA
3	A	134	ILE
3	A	135	GLN
3	A	204	GLY
4	B	350	GLN
3	A	124	ARG
3	A	262	LEU
4	B	476	LEU
3	A	264	ALA
3	A	285	GLU
4	B	427	PRO
4	B	507	LEU
4	B	522	THR
3	A	139	ASN
3	A	208	GLY
4	B	362	PRO
4	B	530	GLU
3	A	66	TYR
4	B	619	VAL
3	A	150	GLY
4	B	469	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	A	223/247 (90%)	209 (94%)	14 (6%)	16	45
4	B	249/269 (93%)	229 (92%)	20 (8%)	11	34
All	All	472/516 (92%)	438 (93%)	34 (7%)	13	39

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	46	ILE
3	A	71	THR
3	A	84	ARG
3	A	96	ARG
3	A	114	GLN
3	A	125	ASP
3	A	139	ASN
3	A	179	LEU
3	A	202	ASN
3	A	224	ILE
3	A	229	THR
3	A	246	ARG
3	A	284	MET
3	A	285	GLU
4	B	345	LEU
4	B	354	ARG
4	B	358	VAL
4	B	387	TYR
4	B	395	VAL
4	B	417	GLU
4	B	420	VAL
4	B	430	MET
4	B	432	VAL
4	B	445	LYS
4	B	468	LEU
4	B	472	ASP
4	B	477	GLN
4	B	490	GLU
4	B	532	VAL
4	B	544	ASN
4	B	552	ARG
4	B	555	ARG
4	B	637	LEU
4	B	641	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	26	GLN
3	A	58	HIS
3	A	64	ASN
3	A	111	HIS
3	A	139	ASN
3	A	162	GLN
3	A	202	ASN
3	A	220	GLN
3	A	241	GLN
3	A	271	GLN
3	A	287	GLN
4	B	350	GLN
4	B	396	GLN
4	B	400	ASN
4	B	441	HIS
4	B	470	HIS
4	B	496	GLN
4	B	544	ASN
4	B	579	GLN
4	B	606	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	C	17/17 (100%)	0.40	1 (5%) 28 21	32, 55, 73, 78	0
2	D	17/17 (100%)	0.26	2 (11%) 9 7	27, 45, 86, 102	0
3	A	275/279 (98%)	0.32	18 (6%) 25 18	22, 45, 85, 103	0
4	B	312/313 (99%)	0.45	35 (11%) 10 7	22, 48, 102, 104	0
All	All	621/626 (99%)	0.39	56 (9%) 15 11	22, 47, 97, 104	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	245	HIS	7.3
4	B	478	ALA	4.7
4	B	479	GLU	4.6
4	B	477	GLN	4.3
4	B	486	LEU	4.2
3	A	99	TYR	4.2
4	B	523	GLY	3.7
4	B	489	ARG	3.7
4	B	463	TYR	3.6
3	A	262	LEU	3.5
2	D	734	DT	3.5
3	A	43	ALA	3.3
4	B	522	THR	3.3
4	B	464	ASN	3.3
3	A	203	SER	3.3
3	A	127	GLU	3.2
4	B	524	SER	3.2
4	B	482	GLY	3.1
4	B	427	PRO	3.1
4	B	487	THR	3.1
3	A	130	ILE	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	B	474	ALA	3.0
3	A	132	GLN	3.0
3	A	55	THR	3.0
4	B	638	GLU	3.0
4	B	426	GLY	2.9
4	B	388	VAL	2.8
4	B	475	TYR	2.8
4	B	490	GLU	2.7
4	B	466	GLY	2.7
3	A	138	ASN	2.7
3	A	49	GLU	2.7
2	D	733	DC	2.7
4	B	483	ASP	2.7
4	B	520	ASP	2.7
3	A	129	ALA	2.6
4	B	467	LEU	2.6
4	B	377	LYS	2.6
4	B	425	ALA	2.6
4	B	521	SER	2.5
4	B	387	TYR	2.4
3	A	54	THR	2.4
1	C	701	DA	2.4
4	B	362	PRO	2.4
4	B	339	GLY	2.3
3	A	53	ASP	2.3
4	B	488	ASP	2.3
4	B	468	LEU	2.2
3	A	291	ASP	2.2
3	A	260	PRO	2.2
4	B	476	LEU	2.1
3	A	18	ALA	2.1
3	A	259	ASP	2.1
4	B	480	GLY	2.1
4	B	484	ARG	2.0
4	B	414	LYS	2.0

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

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.