



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:18 PM UTC

PDB ID : 6PY8 / pdb_00006py8
Title : Crystal structure of the RBPJ-NOTCH1-NRARP ternary complex bound to DNA
Authors : Jarrett, S.M.; Seegar, T.C.M.; Blacklow, S.C.
Deposited on : 2019-07-29
Resolution : 3.75 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
Xtrriage (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

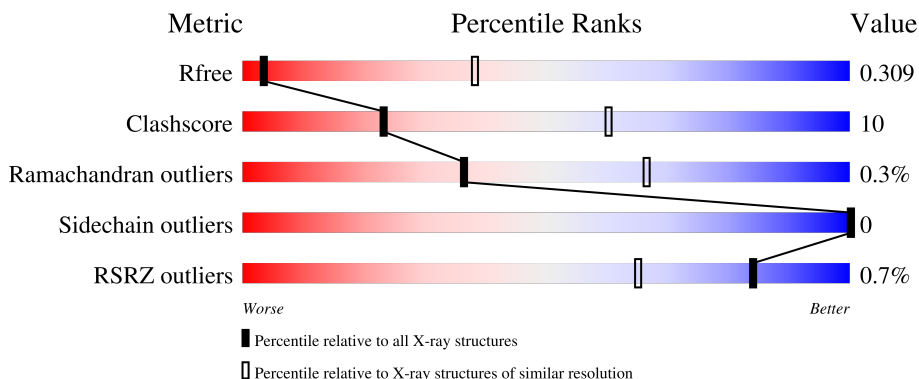
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.75 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	1029 (3.90-3.62)
Clashscore	190562	1061 (3.90-3.62)
Ramachandran outliers	187476	1014 (3.90-3.62)
Sidechain outliers	187428	1009 (3.90-3.62)
RSRZ outliers	180081	1028 (3.90-3.62)

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	B	114	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 69%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 17%; height: 10px; background-color: grey;"></div> </div>
1	G	114	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 63%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 26%; height: 10px; background-color: grey;"></div> </div>
2	A	16	<div style="display: flex; align-items: center;"> <div style="width: 38%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 62%; height: 10px; background-color: yellow;"></div> </div>
2	X	16	<div style="display: flex; align-items: center;"> <div style="width: 38%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 62%; height: 10px; background-color: yellow;"></div> </div>
3	D	16	<div style="display: flex; align-items: center;"> <div style="width: 31%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 69%; height: 10px; background-color: yellow;"></div> </div>

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Mol	Chain	Length	Quality of chain
3	Y	16	 19% 81%
4	C	444	 % 74% 23% .
4	E	444	 68% 28% .
5	F	369	 57% 12% 31%
5	K	369	 53% 17% 30%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 13305 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Notch-regulated ankyrin repeat-containing protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
1	B	95	Total	C	N	O	0	0	0
			642	406	117	119			
1	G	84	Total	C	N	O	0	0	0
			590	375	107	108			

- Molecule 2 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	A	16	Total	C	N	O	P	0	0	0
			333	159	66	93	15			
2	X	16	Total	C	N	O	P	0	0	0
			333	159	66	93	15			

- Molecule 3 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	D	16	Total	C	N	O	P	0	0	0
			317	154	53	95	15			
3	Y	16	Total	C	N	O	P	0	0	0
			317	154	53	95	15			

- Molecule 4 is a protein called Recombining binding protein suppressor of hairless.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	C	429	Total	C	N	O	S	0	0	0
			3408	2157	590	636	25			
4	E	431	Total	C	N	O	S	0	0	0
			3420	2163	592	639	26			

- Molecule 5 is a protein called Neurogenic locus notch homolog protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	F	254	1957	1202	369	378	8	0	0	0
5	K	258	1988	1220	373	387	8	0	0	0

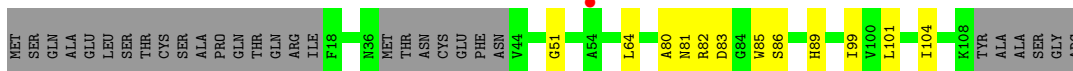
3 Residue-property plots [i](#)

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: Notch-regulated ankyrin repeat-containing protein



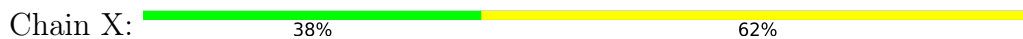
- Molecule 1: Notch-regulated ankyrin repeat-containing protein



- Molecule 2: DNA



- Molecule 2: DNA

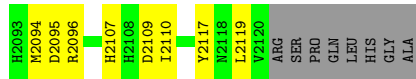


- Molecule 3: DNA

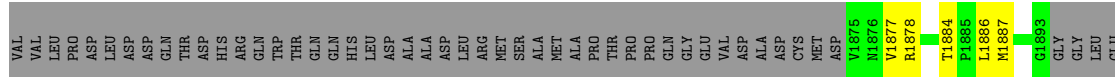
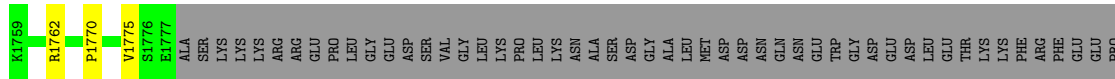


- Molecule 3: DNA





• Molecule 5: Neurogenic locus notch homolog protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.88Å 103.65Å 301.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.46 – 3.75 48.46 – 3.75	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.46-3.75) 93.4 (48.46-3.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 3.77Å)	Xtrriage
Refinement program	PHENIX (1.15.2_3472: ???)	Depositor
R, R_{free}	0.267 , 0.315 0.262 , 0.309	Depositor DCC
R_{free} test set	2000 reflections (7.57%)	wwPDB-VP
Wilson B-factor (Å ²)	103.6	Xtrriage
Anisotropy	0.692	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 53.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13305	wwPDB-VP
Average B, all atoms (Å ²)	119.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% 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	B	0.13	0/651	0.33	0/888
1	G	0.10	0/598	0.25	0/810
2	A	0.13	0/375	0.32	0/579
2	X	0.17	0/375	0.34	0/579
3	D	0.18	0/353	0.40	0/541
3	Y	0.20	0/353	0.42	0/541
4	C	0.12	0/3486	0.34	0/4713
4	E	0.13	0/3498	0.36	0/4729
5	F	0.10	0/1987	0.32	0/2691
5	K	0.11	0/2018	0.33	0/2732
All	All	0.12	0/13694	0.34	0/18803

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	B	642	0	558	13	0
1	G	590	0	545	12	0
2	A	333	0	182	10	0
2	X	333	0	182	9	0
3	D	317	0	183	7	0
3	Y	317	0	183	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	3408	0	3385	71	0
4	E	3420	0	3395	81	0
5	F	1957	0	1886	34	0
5	K	1988	0	1915	47	0
All	All	13305	0	12414	265	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 10.

All (265) 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)
5:F:2091:THR:HB	5:F:2095:ASP:HA	1.65	0.79
4:C:282:MET:HA	4:C:294:PHE:O	1.85	0.76
4:E:279:THR:HG22	4:E:282:MET:HB2	1.71	0.72
5:K:2037:ALA:HA	5:K:2077:THR:HG21	1.70	0.72
5:K:1958:GLN:HB3	5:K:1962:GLY:HA2	1.73	0.70
4:E:333:VAL:HG11	4:E:418:ASP:HB2	1.73	0.70
2:X:4:DA:H2''	2:X:5:DC:H5''	1.72	0.69
4:C:41:VAL:HG21	4:C:268:GLN:HG2	1.75	0.68
4:C:368:LEU:HD11	4:C:414:LEU:HB3	1.75	0.68
4:E:369:ARG:HD3	4:E:376:GLU:HG3	1.76	0.68
2:A:8:DT:H5''	4:E:183:THR:HG22	1.76	0.67
4:C:194:GLY:HA2	4:C:243:MET:HG3	1.77	0.67
5:K:2088:ARG:NH1	5:K:2114:LEU:O	2.29	0.66
4:E:89:ILE:HD13	4:E:129:VAL:HG22	1.79	0.65
5:F:1963:ARG:NH2	5:F:1971:SER:OG	2.29	0.65
4:E:244:ALA:N	5:F:1766:GLN:O	2.30	0.65
4:C:217:GLU:O	4:C:247:ARG:NH1	2.29	0.65
4:C:84:GLN:NE2	4:C:103:LEU:O	2.30	0.64
4:E:282:MET:HA	4:E:294:PHE:O	1.98	0.64
5:F:2054:ASN:HB3	5:F:2057:MET:HG3	1.79	0.64
4:C:384:GLY:N	5:K:2072:GLU:OE2	2.27	0.64
2:A:4:DA:H2''	2:A:5:DC:H5''	1.79	0.63
4:C:367:ASN:HD21	4:C:417:ASN:CG	2.07	0.63
5:F:2037:ALA:HA	5:F:2077:THR:HG21	1.79	0.63
4:C:269:LEU:HD21	4:C:317:ILE:HD12	1.81	0.63
5:K:1906:ASP:HB2	5:K:1909:ALA:HB3	1.81	0.62
4:C:172:LYS:HB3	4:C:205:ALA:HB1	1.81	0.62
4:E:434:PRO:HG3	5:F:1888:ILE:HG12	1.80	0.62
4:E:84:GLN:NE2	4:E:103:LEU:O	2.26	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:324:TYR:HB3	4:E:340:VAL:HG11	1.82	0.62
4:C:324:TYR:HB3	4:C:340:VAL:HG11	1.83	0.61
3:Y:114:DG:H2'	3:Y:115:DT:H71	1.82	0.61
1:G:85:TRP:CH2	4:C:432:PRO:HB2	2.36	0.61
1:G:101:LEU:HA	1:G:104:ILE:HD12	1.82	0.60
4:C:368:LEU:HD21	4:C:414:LEU:HD13	1.84	0.60
1:B:72:LYS:NZ	1:B:72:LYS:O	2.31	0.60
1:G:80:ALA:HA	1:G:86:SER:HA	1.84	0.60
4:C:72:GLN:HA	4:C:75:ARG:HE	1.66	0.60
5:F:1883:PHE:HB3	5:F:1888:ILE:HD11	1.84	0.60
4:C:416:ARG:NH2	4:C:422:TYR:OH	2.35	0.60
2:A:6:DT:H2''	2:A:7:DG:C8	2.36	0.60
1:B:76:ASP:HB3	1:B:79:LEU:HD23	1.85	0.59
4:C:229:HIS:HA	4:C:265:PRO:HA	1.85	0.59
2:X:7:DG:H2''	2:X:8:DT:H5'	1.85	0.59
1:G:85:TRP:HH2	4:C:432:PRO:HB2	1.67	0.58
4:C:172:LYS:HG2	4:C:207:PHE:HE1	1.69	0.58
4:E:104:GLU:HG3	4:E:105:GLY:H	1.69	0.57
4:E:393:ASP:OD1	4:E:394:ILE:N	2.37	0.57
5:K:2107:HIS:HB3	5:K:2110:ILE:HD13	1.86	0.57
5:F:2107:HIS:HB3	5:F:2110:ILE:HD13	1.86	0.57
4:C:293:GLN:HE21	5:K:1770:PRO:HG2	1.69	0.57
5:F:2076:GLU:OE2	5:F:2076:GLU:N	2.31	0.57
5:K:2026:ASP:OD1	5:K:2030:LYS:N	2.36	0.57
5:K:2076:GLU:OE2	5:K:2076:GLU:N	2.31	0.57
5:K:1884:THR:HG22	5:K:1886:LEU:H	1.70	0.56
4:E:216:SER:O	4:E:247:ARG:NH1	2.35	0.56
4:E:337:VAL:HA	4:E:416:ARG:HH22	1.71	0.56
5:F:2013:GLU:HG2	5:F:2047:VAL:HG11	1.88	0.56
1:G:64:LEU:HD23	1:G:99:ILE:HG12	1.88	0.56
4:C:393:ASP:OD1	4:C:394:ILE:N	2.39	0.56
4:C:220:GLU:O	5:K:1762:ARG:NH2	2.39	0.55
4:E:277:LYS:H	4:E:277:LYS:HD3	1.70	0.55
3:D:110:DC:H2''	3:D:111:DA:C8	2.41	0.55
5:F:1959:ASP:OD1	5:F:1963:ARG:N	2.38	0.55
3:D:101:DA:H2'	3:D:102:DA:C8	2.43	0.54
5:F:1963:ARG:HE	5:F:1967:HIS:HB3	1.72	0.54
5:K:1978:PHE:HE2	5:K:2011:MET:HB3	1.73	0.54
3:Y:110:DC:H2''	3:Y:111:DA:C8	2.42	0.53
4:C:69:LYS:HE2	4:C:133:TYR:CZ	2.42	0.53
4:E:291:ILE:HD12	4:E:291:ILE:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:1949:LEU:HD11	5:K:1981:LEU:HD23	1.89	0.53
5:F:1978:PHE:HE2	5:F:2011:MET:HB3	1.73	0.53
5:K:2062:GLU:O	5:K:2092:ASP:HA	2.08	0.53
2:X:11:DG:H1	3:Y:108:DC:H42	1.55	0.53
2:X:3:DG:H1	3:Y:116:DC:H42	1.55	0.53
4:C:327:TYR:HB3	4:C:421:ILE:HG23	1.91	0.53
4:C:54:CYS:SG	4:C:55:PRO:HD3	2.49	0.53
5:F:2037:ALA:HB1	5:F:2069:ALA:HB2	1.90	0.53
4:E:211:LEU:HD11	4:E:235:LYS:HD2	1.91	0.53
5:F:1761:ARG:H	5:F:1761:ARG:HD2	1.74	0.53
5:F:2109:ASP:N	5:F:2109:ASP:OD1	2.41	0.53
4:C:253:VAL:HG12	4:C:258:ALA:HA	1.91	0.52
4:C:22:MET:HE1	4:C:421:ILE:HD13	1.92	0.52
4:E:283:TYR:OH	4:E:314:TRP:HD1	1.92	0.52
4:C:61:LEU:HD21	4:C:131:MET:HE1	1.91	0.52
4:E:49:GLU:OE1	4:E:51:ARG:NH1	2.42	0.52
4:E:373:GLY:N	4:E:411:PRO:O	2.42	0.52
4:E:28:GLU:OE1	4:E:68:LYS:NZ	2.33	0.52
5:K:2091:THR:HB	5:K:2095:ASP:HA	1.92	0.52
4:E:253:VAL:HG12	4:E:258:ALA:HA	1.92	0.52
5:F:2026:ASP:OD1	5:F:2030:LYS:N	2.42	0.52
4:C:35:LEU:HD11	4:C:321:LYS:HE3	1.91	0.51
5:F:1996:GLY:HA3	5:F:2027:ASP:OD2	2.10	0.51
5:F:2087:ASN:HB3	5:F:2090:ILE:HD11	1.92	0.51
1:B:44:VAL:HG22	1:B:45:ASN:H	1.76	0.51
3:D:107:DT:H2''	3:D:108:DC:H5''	1.93	0.51
4:C:347:GLN:HA	5:K:1961:MET:HE1	1.92	0.51
5:F:1992:ARG:NH1	5:F:2025:VAL:O	2.43	0.51
1:B:50:GLU:OE2	4:E:405:ARG:NH2	2.44	0.50
4:E:289:GLU:HG3	4:E:290:ARG:HG2	1.93	0.50
4:E:143:LEU:O	4:E:324:TYR:OH	2.24	0.50
2:A:6:DT:H2''	2:A:7:DG:N7	2.26	0.50
4:E:41:VAL:HG21	4:E:268:GLN:HG2	1.93	0.50
4:E:270:HIS:O	4:E:315:THR:HA	2.12	0.50
4:E:373:GLY:HA2	4:E:411:PRO:HG2	1.94	0.50
4:E:416:ARG:NH2	4:E:422:TYR:OH	2.42	0.50
4:E:29:ARG:NH2	4:E:423:SER:OG	2.45	0.50
2:A:7:DG:H2''	2:A:8:DT:H5'	1.93	0.50
4:C:211:LEU:HD12	4:C:247:ARG:HG2	1.93	0.50
5:K:2068:LEU:HD22	5:K:2071:ARG:HH21	1.76	0.49
2:X:6:DT:H2''	2:X:7:DG:C8	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:14:DA:H2''	2:X:15:DG:H5''	1.94	0.49
4:E:250:ILE:HD12	4:E:266:VAL:HG21	1.92	0.49
5:K:1995:ASP:C	5:K:2027:ASP:HB2	2.36	0.49
4:C:285:CYS:SG	4:C:286:LEU:N	2.86	0.49
4:C:153:PRO:HB3	4:C:269:LEU:HB2	1.93	0.49
5:F:2119:LEU:H	5:F:2119:LEU:HD23	1.78	0.49
5:K:2075:TYR:HE2	5:K:2109:ASP:HB3	1.76	0.49
4:C:367:ASN:C	4:C:367:ASN:HD22	2.21	0.49
5:K:1943:ASP:O	5:K:1947:ARG:NH1	2.45	0.49
3:Y:107:DT:H2''	3:Y:108:DC:H5''	1.94	0.49
5:K:1944:ALA:HA	5:K:1947:ARG:NH2	2.28	0.49
2:A:14:DA:H2''	2:A:15:DG:H5''	1.93	0.49
2:X:10:DG:H2''	2:X:11:DG:C8	2.47	0.49
4:E:153:PRO:HB3	4:E:269:LEU:HB2	1.94	0.49
4:E:251:ARG:HD3	4:E:260:LEU:HB3	1.95	0.49
1:B:71:VAL:HG22	1:B:77:ILE:HD11	1.95	0.49
4:C:280:GLU:N	4:C:280:GLU:OE2	2.46	0.48
4:E:35:LEU:HD11	4:E:321:LYS:HE3	1.95	0.48
3:Y:101:DA:H2'	3:Y:102:DA:C8	2.48	0.48
4:E:346:LEU:HD11	4:E:357:LEU:HD23	1.95	0.48
5:F:2092:ASP:OD1	5:F:2096:ARG:N	2.36	0.48
5:K:1877:VAL:HG12	5:K:1884:THR:HG23	1.95	0.48
1:G:85:TRP:CG	4:C:434:PRO:HB3	2.48	0.48
4:C:392:PRO:O	4:C:430:TYR:OH	2.32	0.48
5:F:2092:ASP:OD2	5:F:2096:ARG:HB2	2.13	0.47
4:C:373:GLY:HA2	4:C:411:PRO:HG2	1.96	0.47
4:E:285:CYS:SG	4:E:286:LEU:N	2.87	0.47
5:K:1992:ARG:NH1	5:K:2025:VAL:O	2.48	0.47
1:G:89:HIS:NE2	5:K:1878:ARG:O	2.44	0.47
4:C:38:HIS:HD2	4:C:147:ILE:HD11	1.79	0.47
4:E:103:LEU:HD21	4:E:109:CYS:HB2	1.96	0.47
1:G:83:ASP:OD2	4:C:405:ARG:HB3	2.14	0.47
4:E:237:VAL:HG22	4:E:244:ALA:HB2	1.96	0.47
4:E:274:PHE:O	4:E:283:TYR:HD1	1.98	0.47
4:E:172:LYS:HG2	4:E:207:PHE:HE1	1.80	0.47
2:A:10:DG:H2''	2:A:11:DG:C8	2.50	0.47
5:F:1884:THR:HG21	5:F:1923:ASN:HD22	1.80	0.47
1:B:52:GLN:HB3	1:B:56:HIS:HB2	1.96	0.46
1:B:67:VAL:O	1:B:71:VAL:HG23	2.15	0.46
4:E:120:ASP:OD2	4:E:122:ARG:NH2	2.47	0.46
4:E:164:ASP:OD2	4:E:164:ASP:N	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:138:ASP:OD1	4:C:139:ILE:N	2.48	0.46
4:E:88:PHE:HB3	4:E:98:MET:HB3	1.97	0.46
4:E:54:CYS:SG	4:E:178:ARG:NH1	2.89	0.46
4:E:251:ARG:O	4:E:273:ALA:N	2.48	0.46
5:K:1959:ASP:OD1	5:K:1963:ARG:N	2.39	0.46
5:K:2092:ASP:OD1	5:K:2096:ARG:N	2.35	0.46
4:E:125:PHE:HA	5:F:2094:MET:HG2	1.96	0.46
4:E:254:ASP:O	4:E:257:THR:OG1	2.33	0.46
4:C:34:VAL:HG21	4:C:142:PHE:HE2	1.80	0.46
4:C:413:THR:HB	4:C:421:ILE:HD11	1.97	0.46
4:E:124:HIS:CD2	4:E:148:LYS:HG3	2.51	0.46
5:K:2092:ASP:OD2	5:K:2096:ARG:HB2	2.16	0.46
4:E:57:PRO:HD2	4:E:111:ALA:O	2.16	0.46
4:E:177:ASN:OD1	4:E:178:ARG:N	2.49	0.46
5:K:1877:VAL:O	5:K:1878:ARG:HG2	2.16	0.45
3:D:105:DT:C6	3:D:106:DT:H72	2.52	0.45
3:Y:114:DG:H2'	3:Y:115:DT:C6	2.51	0.45
2:A:5:DC:H2'	2:A:6:DT:H71	1.98	0.45
5:F:1883:PHE:HD1	5:F:1888:ILE:HG13	1.81	0.45
5:K:1901:SER:N	5:K:1905:GLU:OE2	2.49	0.45
1:B:44:VAL:HG13	1:B:45:ASN:N	2.32	0.45
4:E:34:VAL:HG21	4:E:142:PHE:HE2	1.82	0.45
4:E:138:ASP:OD1	4:E:139:ILE:N	2.50	0.45
4:C:82:GLU:HB3	4:C:135:ASN:HB3	1.98	0.45
4:C:126:MET:HE2	4:C:143:LEU:HB3	1.99	0.45
4:C:178:ARG:HE	4:C:178:ARG:HB2	1.56	0.45
1:G:51:GLY:HA3	1:G:82:ARG:HB2	1.98	0.45
4:E:89:ILE:HG21	4:E:114:LEU:HD11	1.98	0.45
4:E:39:ALA:HA	4:E:319:THR:HA	1.98	0.44
4:E:101:LEU:HD22	4:E:109:CYS:SG	2.57	0.44
4:E:17:LEU:HD21	4:E:22:MET:HB2	1.99	0.44
4:C:286:LEU:HD23	4:C:291:ILE:HG12	1.98	0.44
4:C:383:CYS:SG	4:C:385:GLU:HG2	2.58	0.44
4:C:280:GLU:HG2	5:K:1775:VAL:HG23	1.98	0.44
4:C:342:VAL:O	4:C:361:GLY:HA3	2.17	0.44
3:Y:105:DT:H2'	3:Y:106:DT:H71	1.98	0.44
4:E:230:TYR:CZ	4:E:252:LYS:HB2	2.53	0.44
5:K:1937:ALA:HA	5:K:1977:VAL:HG11	2.00	0.44
1:B:81:ASN:ND2	1:B:85:TRP:O	2.50	0.44
5:F:2062:GLU:O	5:F:2092:ASP:HA	2.18	0.44
1:G:81:ASN:OD1	1:G:85:TRP:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:88:PHE:HD2	4:C:100:GLN:HA	1.83	0.44
5:K:1887:MET:HB3	5:K:1935:LEU:HD12	1.99	0.44
2:X:8:DT:O5'	4:C:178:ARG:NH2	2.51	0.44
3:D:104:DC:H5'	4:E:158:GLN:OE1	2.18	0.43
5:K:2107:HIS:O	5:K:2111:VAL:HG23	2.19	0.43
5:K:1884:THR:HB	5:K:1887:MET:HG3	2.00	0.43
1:B:93:PHE:CD2	4:E:435:GLY:HA3	2.54	0.43
2:A:11:DG:H2''	2:A:12:DA:H8	1.84	0.43
4:E:413:THR:HB	4:E:421:ILE:HD11	1.99	0.43
5:K:1930:GLU:HB3	5:K:1934:HIS:HB2	2.01	0.43
4:E:212:ASP:OD1	4:E:213:ASP:N	2.51	0.43
4:E:327:TYR:HB3	4:E:421:ILE:HG23	2.01	0.43
4:E:333:VAL:HG21	4:E:418:ASP:OD2	2.19	0.43
5:F:1884:THR:O	5:F:1888:ILE:HD12	2.19	0.43
5:K:2058:GLN:HB2	5:K:2062:GLU:HA	2.00	0.43
5:F:2088:ARG:NH2	5:F:2117:TYR:O	2.33	0.42
4:C:172:LYS:HG2	4:C:207:PHE:CE1	2.50	0.42
4:E:215:GLU:OE1	4:E:222:THR:N	2.51	0.42
5:K:1907:ALA:N	5:K:1908:PRO:HD2	2.34	0.42
5:K:1966:LEU:HD11	5:K:1978:PHE:CE1	2.55	0.42
4:E:248:LEU:HB3	4:E:274:PHE:HB3	2.01	0.42
4:E:283:TYR:CE2	4:E:312:ALA:HB1	2.54	0.42
4:C:279:THR:HG23	5:K:1775:VAL:HG21	2.01	0.42
5:K:2112:ARG:O	5:K:2116:GLU:HG2	2.19	0.42
4:C:12:PRO:HA	4:C:13:PRO:HD3	1.88	0.42
4:E:38:HIS:HD2	4:E:147:ILE:HD11	1.83	0.42
5:F:2054:ASN:CB	5:F:2057:MET:HG3	2.47	0.42
4:C:403:TRP:CD1	4:C:436:PRO:HB3	2.55	0.42
3:D:113:DA:H2''	3:D:114:DG:C8	2.55	0.42
4:C:80:GLU:HB2	4:E:225:ASP:HB3	2.01	0.42
4:C:221:PHE:CE1	4:C:235:LYS:HD3	2.55	0.42
4:C:373:GLY:N	4:C:411:PRO:O	2.52	0.42
4:E:44:LYS:HG2	4:E:151:SER:HA	2.02	0.42
5:K:1978:PHE:O	5:K:1982:ILE:HG12	2.19	0.42
1:B:77:ILE:HD13	1:B:77:ILE:HA	1.89	0.42
4:E:177:ASN:HD21	4:E:311:GLY:C	2.28	0.42
4:E:412:VAL:O	4:E:424:THR:OG1	2.31	0.42
5:K:1906:ASP:OD1	5:K:1906:ASP:N	2.42	0.42
1:B:55:LEU:CD1	1:B:67:VAL:HG23	2.50	0.41
4:E:250:ILE:H	4:E:250:ILE:HG12	1.71	0.41
5:K:1884:THR:HG22	5:K:1886:LEU:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:85:TRP:CD1	4:C:434:PRO:HB3	2.55	0.41
4:E:141:VAL:O	4:E:338:THR:OG1	2.35	0.41
4:E:330:MET:HB2	4:E:419:GLY:HA3	2.02	0.41
5:K:2054:ASN:HB3	5:K:2057:MET:HB2	2.01	0.41
4:C:58:CYS:SG	4:C:203:TRP:NE1	2.93	0.41
4:C:69:LYS:O	4:C:69:LYS:HD3	2.20	0.41
5:F:2064:THR:HG23	5:F:2067:PHE:H	1.85	0.41
1:B:56:HIS:O	1:B:60:ILE:HG13	2.20	0.41
4:E:99:GLN:NE2	4:E:113:THR:O	2.43	0.41
4:E:254:ASP:OD1	4:E:254:ASP:N	2.53	0.41
4:E:384:GLY:H	5:F:2072:GLU:CD	2.29	0.41
2:X:8:DT:O3'	4:C:178:ARG:HD2	2.21	0.41
4:E:383:CYS:SG	4:E:385:GLU:HG2	2.61	0.41
3:D:107:DT:OP2	4:E:46:TYR:HE1	2.04	0.41
4:C:254:ASP:OD1	4:C:254:ASP:N	2.53	0.41
5:F:1943:ASP:OD1	5:F:1943:ASP:N	2.52	0.41
4:C:189:LEU:HD21	4:C:196:PHE:HD2	1.86	0.41
4:E:230:TYR:OH	4:E:270:HIS:ND1	2.46	0.41
5:K:1943:ASP:N	5:K:1943:ASP:OD1	2.51	0.41
4:C:271:LYS:HE3	4:C:271:LYS:HB2	1.88	0.41
2:A:7:DG:H5'	4:E:52:PHE:CZ	2.56	0.40
3:Y:112:DC:H2'	3:Y:113:DA:C8	2.56	0.40
4:C:210:LEU:HD22	4:C:224:ARG:HE	1.86	0.40
4:C:385:GLU:OE2	5:K:2030:LYS:NZ	2.48	0.40
5:K:1942:SER:HB3	5:K:1980:ILE:HD12	2.02	0.40
4:C:177:ASN:OD1	4:C:178:ARG:N	2.53	0.40
4:C:249:ILE:HD12	4:C:275:TYR:HD2	1.87	0.40
4:C:288:GLN:O	4:C:289:GLU:HB2	2.21	0.40
1:G:86:SER:OG	1:G:89:HIS:ND1	2.53	0.40
4:C:267:SER:H	4:C:270:HIS:CE1	2.40	0.40
5:F:1995:ASP:OD1	5:F:1995:ASP:N	2.47	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	93/114 (82%)	86 (92%)	6 (6%)	1 (1%)	11	40
1	G	80/114 (70%)	72 (90%)	8 (10%)	0	100	100
4	C	427/444 (96%)	393 (92%)	34 (8%)	0	100	100
4	E	429/444 (97%)	391 (91%)	34 (8%)	4 (1%)	14	43
5	F	248/369 (67%)	233 (94%)	15 (6%)	0	100	100
5	K	252/369 (68%)	237 (94%)	15 (6%)	0	100	100
All	All	1529/1854 (82%)	1412 (92%)	112 (7%)	5 (0%)	36	66

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	E	97	GLU
4	E	436	PRO
1	B	44	VAL
4	E	282	MET
4	E	288	GLN

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	50/93 (54%)	50 (100%)	0	100	100
1	G	51/93 (55%)	51 (100%)	0	100	100
4	C	378/387 (98%)	378 (100%)	0	100	100
4	E	380/387 (98%)	380 (100%)	0	100	100
5	F	200/302 (66%)	200 (100%)	0	100	100
5	K	204/302 (68%)	204 (100%)	0	100	100
All	All	1263/1564 (81%)	1263 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	63	ASN
4	C	32	GLN
4	C	124	HIS
4	C	135	ASN
4	C	158	GLN
4	C	304	ASN
4	C	367	ASN
4	E	32	GLN
4	E	96	GLN
4	E	124	HIS
4	E	182	GLN
4	E	190	HIS
4	E	209	HIS
4	E	309	ASN
4	E	349	ASN
5	F	1984	ASN
5	F	2041	ASN
5	K	1975	GLN
5	K	1984	ASN
5	K	2093	HIS
5	K	2103	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 i

6.1 Protein, DNA and RNA chains i

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	B	95/114 (83%)	0.52	4 (4%) 40 28	92, 129, 228, 254	0
1	G	84/114 (73%)	0.00	1 (1%) 76 54	98, 131, 151, 159	0
2	A	16/16 (100%)	-0.16	0 100 100	125, 148, 165, 165	0
2	X	16/16 (100%)	-0.07	0 100 100	109, 146, 165, 166	0
3	D	16/16 (100%)	-0.17	0 100 100	116, 145, 162, 163	0
3	Y	16/16 (100%)	-0.23	0 100 100	107, 134, 168, 177	0
4	C	429/444 (96%)	0.01	3 (0%) 84 65	69, 105, 148, 175	1 (0%)
4	E	431/444 (97%)	-0.03	2 (0%) 87 70	65, 116, 163, 192	1 (0%)
5	F	254/369 (68%)	-0.01	0 100 100	79, 107, 160, 204	0
5	K	258/369 (69%)	-0.10	1 (0%) 88 73	80, 111, 141, 162	0
All	All	1615/1918 (84%)	0.00	11 (0%) 84 65	65, 114, 162, 254	2 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	98	ASP	3.5
1	B	102	TYR	2.7
4	C	141	VAL	2.6
4	E	58	CYS	2.5
1	G	54	ALA	2.4
5	K	2014	ASP	2.4
4	C	54	CYS	2.3
1	B	19	GLN	2.2
4	E	156	LYS	2.1
1	B	99	ILE	2.0
4	C	140	GLY	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.