



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 02:16 AM GMT

PDB ID : 3C25
Title : Crystal Structure of NotI Restriction Endonuclease Bound to Cognate DNA
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Deposited on : 2008-01-24
Resolution : 2.50 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

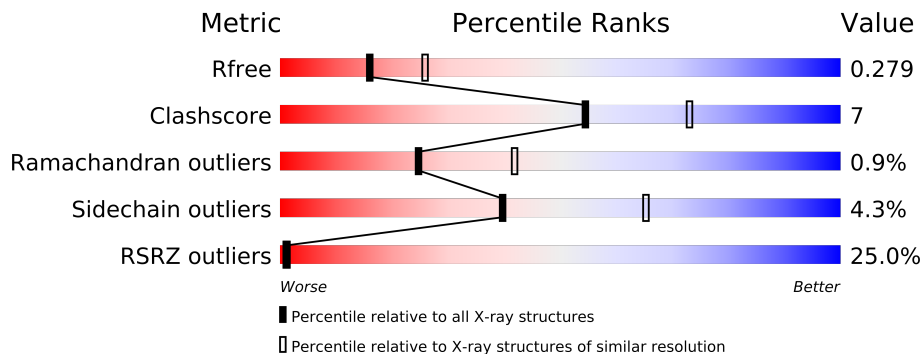
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance



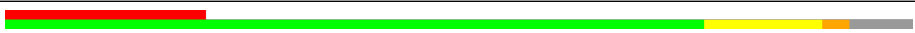
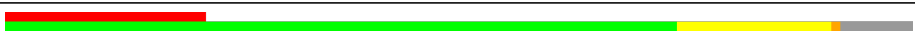
The reported resolution of this entry is 2.50 Å.

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}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	C	22	
2	D	22	
3	A	383	
3	B	383	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	FE	B	902	-	X
5	CA	B	804	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6508 atoms, of which 0 are hydrogen and 0 are deuterium.

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 DNA (5'-D(*DCP*DGP*DGP*DAP*DGP*DGP*DCP*DGP*DCP*DGP*DGP*DCP*DCP*DGP*DCP*DCP*DCP*DCP*DG)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	22	Total	C	N	O	P	0	0	0
			450	210	90	129	21			

- Molecule 2 is a DNA chain called DNA (5'-D(*DCP*DGP*DGP*DCP*DGP*DGP*DCP*DGP*DCP*DGP*DGP*DCP*DCP*DGP*DCP*DCP*DTP*DCP*DCP*DG)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	22	Total	C	N	O	P	0	0	0
			446	209	85	131	21			

- Molecule 3 is a protein called NotI restriction endonuclease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	354	Total	C	N	O	S	0	0	0
			2720	1743	469	498	10			
3	B	353	Total	C	N	O	S	0	0	0
			2718	1740	467	501	10			

- Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe).

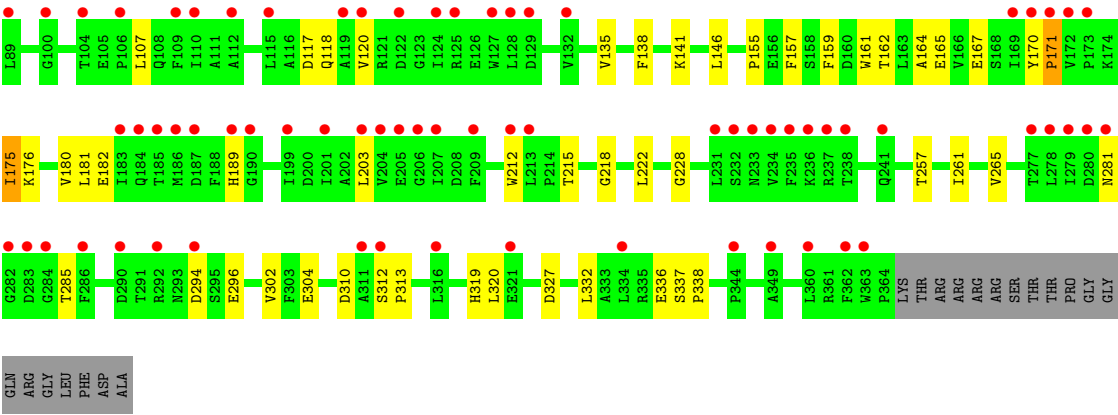
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Fe	0	0
			1	1		
4	A	1	Total	Fe	0	0
			1	1		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Ca	0	0
			2	2		
5	A	2	Total	Ca	0	0
			2	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	56	Total	O	0	0
			56	56		
6	B	60	Total	O	0	0
			60	60		
6	C	25	Total	O	0	0
			25	25		
6	D	27	Total	O	0	0
			27	27		



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.89Å 81.71Å 73.58Å 90.00° 99.51° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 47.64 – 2.49	Depositor EDS
% Data completeness (in resolution range)	97.7 (50.00-2.50) 97.3 (47.64-2.49)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.68 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.223 , 0.277 0.225 , 0.279	Depositor DCC
R_{free} test set	1488 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	55.3	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 74.1	EDS
Estimated twinning fraction	0.017 for l,-k,h	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	6 of 29457 reflections (0.020%)	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6508	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.46 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.3178e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, FE

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	0.62	0/505	1.27	5/778 (0.6%)
2	D	0.63	0/499	1.16	3/768 (0.4%)
3	A	0.39	2/2795 (0.1%)	0.51	0/3812
3	B	0.37	0/2793	0.51	0/3809
All	All	0.43	2/6592 (0.0%)	0.68	8/9167 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	42	CYS	CB-SG	5.73	1.92	1.82
3	A	65	CYS	CB-SG	5.56	1.91	1.82

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1	DC	O3'-P-O5'	-11.24	82.64	104.00
1	C	1	DC	OP2-P-O3'	-8.04	87.51	105.20
1	C	1	DC	OP1-P-O3'	-7.88	87.86	105.20
1	C	10	DG	O4'-C1'-N9	7.45	113.22	108.00
2	D	10	DG	O4'-C1'-N9	6.64	112.65	108.00
2	D	1	DC	O4'-C1'-N1	6.38	112.47	108.00
2	D	3	DG	P-O3'-C3'	6.36	127.33	119.70
1	C	2	DG	OP1-P-OP2	5.17	127.35	119.60

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	450	0	244	3	0
2	D	446	0	245	3	0
3	A	2720	0	2615	42	0
3	B	2718	0	2614	38	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	56	0	0	0	0
6	B	60	0	0	1	0
6	C	25	0	0	0	0
6	D	27	0	0	0	0
All	All	6508	0	5718	82	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (82) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:29:SER:CB	3:A:210:HIS:CE1	1.91	1.53
3:A:29:SER:CB	3:A:210:HIS:ND1	1.97	1.24
3:A:283:ASP:OD1	3:A:285:THR:HG22	1.40	1.16
3:A:283:ASP:CG	3:A:285:THR:HG22	1.76	1.05
3:A:29:SER:CB	3:A:210:HIS:HE1	1.61	0.91
3:A:312:SER:HB2	3:A:313:PRO:HD3	1.53	0.89
3:B:180:VAL:HB	3:B:257:THR:HG22	1.60	0.83
3:A:283:ASP:OD1	3:A:285:THR:CG2	2.26	0.82
3:A:27:VAL:O	3:A:27:VAL:HG12	1.83	0.77
2:D:8:DG:N7	3:B:189:HIS:HE1	1.84	0.76
3:A:79:LEU:HD13	3:A:84:ARG:HG3	1.70	0.73
3:B:212:TRP:O	3:B:215:THR:HG22	1.95	0.67
3:B:16:ALA:HB3	3:B:66:VAL:HG12	1.78	0.66
3:B:167:GLU:HB3	3:B:176:LYS:HG3	1.78	0.65
3:B:80:VAL:HG12	3:B:80:VAL:O	1.96	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:212:TRP:O	3:A:215:THR:HG22	1.97	0.64
3:A:283:ASP:OD2	3:A:285:THR:HG22	2.02	0.60
1:C:8:DG:N7	3:A:189:HIS:HE1	1.99	0.60
3:B:332:LEU:HA	3:B:336:GLU:HB2	1.84	0.60
3:A:309:THR:HG21	3:A:315:PRO:HD2	1.83	0.59
3:B:138:PHE:HB2	3:B:162:THR:HG23	1.84	0.59
3:A:117:ASP:HB3	3:A:120:VAL:HG22	1.85	0.58
3:B:24:TYR:HB3	3:B:25:PRO:HD3	1.86	0.58
3:A:283:ASP:CG	3:A:285:THR:CG2	2.64	0.57
3:B:161:TRP:HB2	3:B:181:LEU:HB2	1.86	0.56
3:B:215:THR:HG23	3:B:218:GLY:H	1.72	0.55
3:B:41:THR:HA	3:B:54:SER:HA	1.89	0.54
3:B:312:SER:OG	3:B:313:PRO:HD3	2.07	0.54
3:A:24:TYR:HB3	3:A:25:PRO:HD3	1.90	0.54
3:A:283:ASP:OD2	3:A:285:THR:CG2	2.55	0.54
3:A:161:TRP:HB2	3:A:181:LEU:HB2	1.89	0.54
3:A:170:TYR:CB	3:A:171:PRO:HD3	2.39	0.53
3:B:56:VAL:HG11	3:B:141:LYS:HE2	1.92	0.52
3:A:281:ASN:HD22	3:A:285:THR:HG23	1.75	0.52
3:A:34:ARG:HH12	3:A:209:PHE:H	1.56	0.52
3:A:332:LEU:HA	3:A:336:GLU:HB2	1.91	0.51
3:B:17:GLU:HG2	3:B:66:VAL:HB	1.92	0.51
3:A:281:ASN:HD21	3:A:287:SER:HB2	1.74	0.51
3:B:138:PHE:HB2	3:B:162:THR:CG2	2.41	0.51
3:B:21:HIS:CE1	3:B:312:SER:HB2	2.46	0.50
3:A:312:SER:CB	3:A:313:PRO:HD3	2.35	0.50
3:B:162:THR:HG22	6:B:929:HOH:O	2.10	0.50
3:A:312:SER:HB2	3:A:313:PRO:CD	2.35	0.50
3:B:16:ALA:HB2	3:B:68:ASN:HB2	1.92	0.49
3:B:17:GLU:HA	3:B:23:VAL:HG22	1.94	0.49
3:A:22:ARG:HD2	3:A:25:PRO:HD2	1.95	0.49
3:A:114:THR:HG22	3:A:120:VAL:HG21	1.95	0.49
3:B:164:ALA:HB1	3:B:175:ILE:HG21	1.95	0.48
3:A:97:LYS:HG3	3:A:299:TRP:CZ2	2.49	0.48
3:A:70:ALA:HB2	3:A:75:ARG:HE	1.78	0.48
3:A:41:THR:HA	3:A:54:SER:HA	1.96	0.47
3:B:159:PHE:HA	3:B:182:GLU:OE2	2.15	0.47
3:B:337:SER:HB3	3:B:338:PRO:HD3	1.96	0.47
3:B:302:VAL:HB	3:B:320:LEU:HB3	1.96	0.46
2:D:8:DG:N7	3:B:189:HIS:CE1	2.74	0.46
3:A:79:LEU:HD13	3:A:84:ARG:CG	2.42	0.45
1:C:13:DC:H2'	1:C:14:DG:C8	2.52	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:B:189:HIS:HD2	3:B:228:GLY:O	2.01	0.44
3:A:215:THR:OG1	3:A:216:PRO:HD2	2.17	0.44
3:A:38:ALA:HA	3:A:203:LEU:HD21	1.99	0.44
3:A:151:THR:HG22	3:A:152:ASP:H	1.82	0.44
3:A:80:VAL:O	3:A:80:VAL:CG1	2.64	0.44
3:B:281:ASN:HB2	3:B:285:THR:HG23	1.98	0.44
2:D:11:DG:N7	3:A:237:ARG:NH2	2.62	0.44
3:A:302:VAL:HB	3:A:320:LEU:HB3	1.99	0.43
3:B:15:ILE:HB	3:B:222:LEU:HD12	1.99	0.43
3:B:261:ILE:HB	3:B:265:VAL:CG2	2.48	0.43
3:A:189:HIS:HD2	3:A:228:GLY:O	2.02	0.43
3:B:117:ASP:HB2	3:B:120:VAL:HG22	2.00	0.43
3:A:27:VAL:O	3:A:27:VAL:CG1	2.56	0.42
1:C:18:DC:H2"	1:C:19:DG:C8	2.54	0.42
3:B:155:PRO:HG2	3:B:157:PHE:CE2	2.55	0.42
3:B:38:ALA:HA	3:B:203:LEU:HD21	2.01	0.42
3:B:304:GLU:HG3	3:B:319:HIS:HB2	2.01	0.42
3:B:69:THR:HB	3:B:78:TRP:HE1	1.85	0.41
3:A:110:ILE:H	3:A:110:ILE:HD13	1.85	0.41
3:B:135:VAL:HG12	3:B:165:GLU:HA	2.02	0.41
3:A:304:GLU:HG3	3:A:319:HIS:HB2	2.02	0.41
3:B:41:THR:HG23	3:B:53:THR:O	2.21	0.41
3:B:146:LEU:HB2	3:B:162:THR:HG21	2.02	0.41
3:A:337:SER:HB3	3:A:338:PRO:HD3	2.02	0.41
3:B:170:TYR:CB	3:B:171:PRO:HD3	2.51	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	
3	A	352/383 (92%)	329 (94%)	20 (6%)	3 (1%)	25	42
3	B	351/383 (92%)	328 (93%)	20 (6%)	3 (1%)	25	42
All	All	703/766 (92%)	657 (94%)	40 (6%)	6 (1%)	25	42

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	28	VAL
3	B	294	ASP
3	A	171	PRO
3	A	24	TYR
3	B	171	PRO
3	B	24	TYR

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	278/317 (88%)	264 (95%)	14 (5%)	34	58
3	B	280/317 (88%)	270 (96%)	10 (4%)	47	73
All	All	558/634 (88%)	534 (96%)	24 (4%)	40	65

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	22	ARG
3	A	42	CYS
3	A	55	CYS
3	A	62	ARG
3	A	75	ARG
3	A	79	LEU
3	A	97	LYS
3	A	110	ILE
3	A	118	GLN
3	A	151	THR
3	A	177	ARG
3	A	193	LYS
3	A	234	VAL
3	A	287	SER
3	B	42	CYS
3	B	55	CYS
3	B	71	VAL
3	B	75	ARG

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Mol	Chain	Res	Type
3	B	107	LEU
3	B	118	GLN
3	B	175	ILE
3	B	296	GLU
3	B	310	ASP
3	B	327	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	184	GLN
3	A	189	HIS
3	A	281	ASN
3	B	118	GLN
3	B	189	HIS
3	B	281	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	C	22/22 (100%)	1.34	7 (31%) 1 1	56, 61, 72, 76	0
2	D	22/22 (100%)	1.36	6 (27%) 1 1	57, 63, 76, 78	0
3	A	354/383 (92%)	1.37	86 (24%) 1 1	26, 67, 72, 77	0
3	B	353/383 (92%)	1.45	86 (24%) 1 1	58, 67, 72, 76	0
All	All	751/810 (92%)	1.41	185 (24%) 1 1	26, 67, 72, 78	0

All (185) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	204	VAL	8.4
3	B	32	ALA	8.1
3	A	312	SER	8.1
3	A	104	THR	6.4
3	B	203	LEU	6.4
3	B	104	THR	5.7
3	A	127	TRP	5.6
3	A	120	VAL	5.5
3	A	166	VAL	5.3
3	A	172	VAL	5.3
3	A	169	ILE	5.2
3	B	278	LEU	5.2
3	B	281	ASN	5.1
3	A	207	ILE	5.0
3	A	284	GLY	4.9
3	B	119	ALA	4.8
3	A	295	SER	4.8
2	D	1	DC	4.7
3	B	363	TRP	4.6
3	B	106	PRO	4.6
3	B	312	SER	4.5

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Mol	Chain	Res	Type	RSRZ
3	A	282	GLY	4.4
3	A	65	CYS	4.4
3	B	205	GLU	4.3
3	B	170	TYR	4.3
3	B	29	SER	4.3
3	B	129	ASP	4.2
3	A	279	ILE	4.2
3	A	55	CYS	4.1
3	B	55	CYS	4.0
3	B	132	VAL	4.0
3	B	127	TRP	4.0
1	C	11	DG	4.0
3	A	110	ILE	4.0
3	B	124	ILE	4.0
3	A	283	ASP	4.0
3	B	277	THR	4.0
3	B	283	ASP	4.0
3	B	284	GLY	3.9
3	B	213	LEU	3.9
1	C	10	DG	3.9
3	B	172	VAL	3.9
3	B	238	THR	3.9
3	A	363	TRP	3.9
3	B	234	VAL	3.8
3	A	235	PHE	3.8
3	A	278	LEU	3.8
3	A	234	VAL	3.8
2	D	11	DG	3.8
3	B	280	ASP	3.8
3	B	279	ILE	3.8
3	A	345	SER	3.7
3	B	362	PHE	3.7
3	A	238	THR	3.7
3	B	33	ALA	3.7
2	D	10	DG	3.7
3	A	81	CYS	3.7
3	A	237	ARG	3.7
3	B	24	TYR	3.7
3	B	81	CYS	3.7
3	B	185	THR	3.6
3	A	124	ILE	3.6
3	A	125	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	1	DC	3.6
3	B	115	LEU	3.5
3	A	236	LYS	3.5
3	B	209	PHE	3.5
3	B	237	ARG	3.5
3	A	129	ASP	3.5
3	B	80	VAL	3.4
3	A	122	ASP	3.4
3	B	42	CYS	3.4
3	A	24	TYR	3.4
3	A	231	LEU	3.4
3	A	233	ASN	3.3
3	B	128	LEU	3.3
3	B	65	CYS	3.3
3	A	293	ASN	3.3
3	B	294	ASP	3.3
3	A	119	ALA	3.2
3	A	344	PRO	3.2
3	B	20	GLY	3.2
3	B	235	PHE	3.2
3	B	25	PRO	3.2
3	A	116	ALA	3.1
3	A	190	GLY	3.1
3	A	174	LYS	3.1
3	A	113	PRO	3.1
3	B	207	ILE	3.1
3	A	34	ARG	3.0
3	A	80	VAL	3.0
3	A	232	SER	3.0
3	B	190	GLY	3.0
1	C	8	DG	3.0
3	A	132	VAL	3.0
3	A	277	THR	3.0
3	B	183	ILE	2.9
3	B	31	GLU	2.9
1	C	9	DC	2.9
3	B	236	LYS	2.9
3	A	186	MET	2.9
3	B	189	HIS	2.9
3	B	212	TRP	2.9
3	B	186	MET	2.8
1	C	22	DG	2.8

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Mol	Chain	Res	Type	RSRZ
3	A	126	GLU	2.8
3	B	233	ASN	2.8
3	B	125	ARG	2.8
3	B	120	VAL	2.8
3	A	185	THR	2.8
3	B	169	ILE	2.8
3	A	189	HIS	2.8
3	A	134	VAL	2.8
3	A	205	GLU	2.8
3	A	311	ALA	2.8
3	A	107	LEU	2.8
3	A	103	PRO	2.7
3	A	149	SER	2.7
3	B	122	ASP	2.7
3	A	31	GLU	2.7
3	A	123	GLY	2.7
3	B	100	GLY	2.7
3	A	35	ASN	2.7
3	B	74	GLU	2.6
3	A	42	CYS	2.6
3	A	181	LEU	2.6
2	D	9	DC	2.6
3	A	188	PHE	2.6
3	A	29	SER	2.6
3	A	301	PHE	2.6
3	B	321	GLU	2.6
3	A	187	ASP	2.6
3	A	184	GLN	2.5
3	B	187	ASP	2.5
3	A	157	PHE	2.5
3	B	206	GLY	2.5
3	A	147	SER	2.5
3	B	231	LEU	2.5
3	A	240	TYR	2.4
3	B	109	PHE	2.4
3	A	230	ASN	2.4
3	A	256	GLY	2.4
3	A	285	THR	2.4
3	B	89	LEU	2.4
3	A	183	ILE	2.4
3	A	23	VAL	2.4
3	B	50	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
3	A	212	TRP	2.3
3	B	232	SER	2.3
3	A	281	ASN	2.3
3	A	171	PRO	2.3
3	B	241	GLN	2.3
3	B	199	ILE	2.3
3	A	265	VAL	2.3
3	A	241	GLN	2.3
3	A	364	PRO	2.3
3	B	171	PRO	2.3
2	D	8	DG	2.2
3	A	131	GLY	2.2
3	B	360	LEU	2.2
3	A	192	TYR	2.2
3	B	184	GLN	2.2
3	B	286	PHE	2.2
3	B	282	GLY	2.2
3	B	311	ALA	2.2
3	A	239	PHE	2.1
3	A	268	SER	2.1
3	B	173	PRO	2.1
3	A	208	ASP	2.1
3	B	16	ALA	2.1
3	A	323	ARG	2.1
3	B	316	LEU	2.1
3	B	112	ALA	2.1
2	D	22	DG	2.1
3	A	173	PRO	2.1
1	C	7	DC	2.1
3	B	110	ILE	2.1
3	B	334	LEU	2.1
3	B	292	ARG	2.0
3	B	349	ALA	2.0
3	A	109	PHE	2.0
3	B	290	ASP	2.0
3	B	201	ILE	2.0
3	B	344	PRO	2.0
3	B	85	ALA	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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	CA	B	804	1/1	0.60	4.74	89,89,89,89	0
4	FE	B	902	1/1	0.36	2.06	64,64,64,64	0
4	FE	A	901	1/1	0.37	1.74	64,64,64,64	0
5	CA	A	802	1/1	0.27	-0.86	97,97,97,97	0
5	CA	B	803	1/1	0.23	-0.96	115,115,115,115	0
5	CA	A	801	1/1	0.20	-1.68	103,103,103,103	0

6.5 Other polymers ⓘ

There are no such residues in this entry.