



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 02:12 am BST

PDB ID : 3C25
Title : Crystal Structure of NotI Restriction Endonuclease Bound to Cognate DNA
Authors : Lambert, A.R.; Sussman, D.; Shen, B.; Stoddard, B.L.
Deposited on : 2008-01-24
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

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

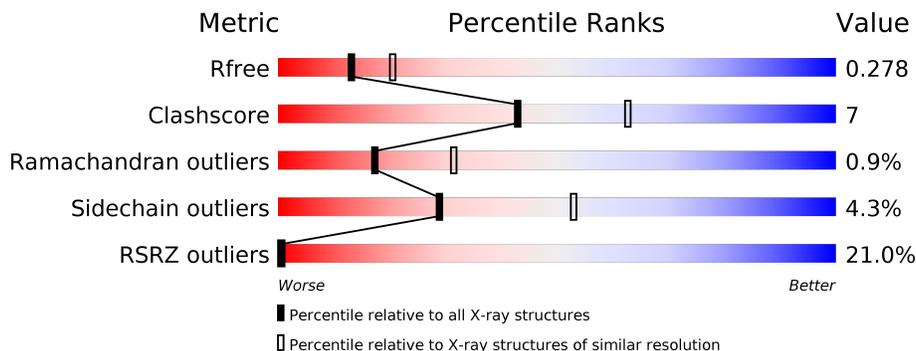
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

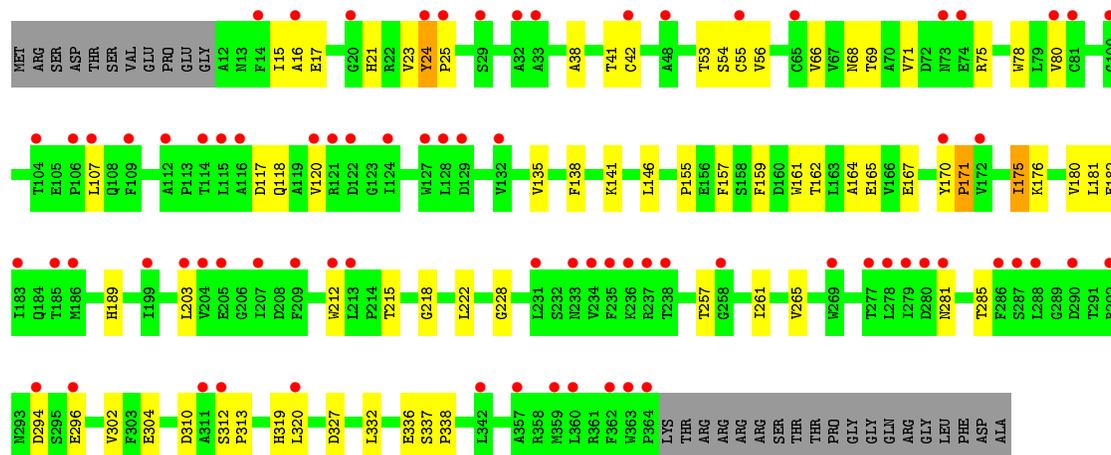
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	22	18% (Poor fit) 64% (0 outliers) 36% (1 outlier)
2	D	22	23% (Poor fit) 77% (0 outliers) 23% (1 outlier)
3	A	383	19% (Poor fit) 77% (0 outliers) 13% (1 outlier) 8% (2 outliers)
3	B	383	20% (Poor fit) 74% (0 outliers) 17% (1 outlier) 8% (2 outliers)

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

- Molecule 6 is water.

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



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)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.223 , 0.277 0.224 , 0.278	Depositor DCC
R_{free} test set	1488 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	55.3	Xtrriage
Anisotropy	0.349	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 54.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.017 for l,-k,h	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6508	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtrriage'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.*

¹ Intensities estimated from amplitudes.

² Theoretical 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

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 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	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

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 7.

All (82) 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)
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	Interatomic distance (Å)	Clash overlap (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:A:24:TYR:HB3	3:A:25:PRO:HD3	1.90	0.54
3:B:312:SER:OG	3:B:313:PRO:HD3	2.07	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:DC:H2'	1:C:14:DG:C8	2.52	0.45
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:B:189:HIS:HD2	3:B:228:GLY:O	2.01	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:A:110:ILE:H	3:A:110:ILE:HD13	1.85	0.41
3:B:69:THR:HB	3:B:78:TRP:HE1	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 [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	352/383 (92%)	329 (94%)	20 (6%)	3 (1%)	17	31
3	B	351/383 (92%)	328 (93%)	20 (6%)	3 (1%)	17	31
All	All	703/766 (92%)	657 (94%)	40 (6%)	6 (1%)	17	31

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 [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	
3	A	278/317 (88%)	264 (95%)	14 (5%)	24	46
3	B	280/317 (88%)	270 (96%)	10 (4%)	35	61
All	All	558/634 (88%)	534 (96%)	24 (4%)	29	53

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

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Mol	Chain	Res	Type
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
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 [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 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.

No monomer is involved in short contacts.

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 [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	C	22/22 (100%)	1.16	4 (18%) 1 1	56, 61, 72, 76	0
2	D	22/22 (100%)	1.26	5 (22%) 0 0	57, 63, 76, 78	0
3	A	354/383 (92%)	1.23	72 (20%) 1 0	26, 67, 72, 77	0
3	B	353/383 (92%)	1.30	77 (21%) 0 0	58, 67, 72, 76	0
All	All	751/810 (92%)	1.26	158 (21%) 1 0	26, 67, 72, 78	0

All (158) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	204	VAL	9.3
3	A	166	VAL	8.8
3	B	124	ILE	8.3
3	A	207	ILE	7.7
3	B	32	ALA	7.1
3	A	312	SER	7.0
3	B	199	ILE	6.9
3	A	120	VAL	6.7
3	A	127	TRP	6.4
3	A	284	GLY	6.3
3	A	172	VAL	6.3
3	A	104	THR	6.0
3	A	122	ASP	5.6
3	B	294	ASP	5.5
3	B	172	VAL	5.5
3	A	24	TYR	5.3
3	B	203	LEU	5.3
3	B	100	GLY	5.1
3	A	119	ALA	5.1
3	B	104	THR	5.0
3	B	129	ASP	4.9

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Mol	Chain	Res	Type	RSRZ
3	B	115	LEU	4.8
3	A	205	GLU	4.8
3	B	106	PRO	4.8
3	A	132	VAL	4.8
3	B	213	LEU	4.7
3	A	123	GLY	4.7
3	A	364	PRO	4.7
3	B	170	TYR	4.7
3	B	363	TRP	4.6
3	A	65	CYS	4.5
3	B	25	PRO	4.5
3	A	169	ILE	4.5
3	B	234	VAL	4.5
2	D	1	DC	4.4
3	B	312	SER	4.4
3	A	282	GLY	4.4
3	A	363	TRP	4.3
3	B	55	CYS	4.3
3	B	281	ASN	4.2
3	B	280	ASP	4.1
3	B	128	LEU	4.0
3	B	238	THR	4.0
3	B	29	SER	3.9
3	B	20	GLY	3.9
3	A	204	VAL	3.9
3	A	283	ASP	3.8
3	A	293	ASN	3.8
3	A	201	ILE	3.8
3	B	279	ILE	3.6
3	A	55	CYS	3.6
3	A	344	PRO	3.6
3	B	120	VAL	3.6
3	B	362	PHE	3.5
3	B	235	PHE	3.5
3	A	134	VAL	3.5
3	B	121	ARG	3.4
3	B	33	ALA	3.4
3	B	364	PRO	3.4
3	A	345	SER	3.4
3	B	209	PHE	3.4
3	B	292	ARG	3.4
3	A	237	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
3	A	234	VAL	3.3
3	B	360	LEU	3.3
3	B	80	VAL	3.3
3	A	279	ILE	3.2
3	B	231	LEU	3.2
3	B	65	CYS	3.2
3	B	278	LEU	3.2
3	B	237	ARG	3.2
3	A	124	ILE	3.1
3	B	24	TYR	3.1
3	B	42	CYS	3.1
3	B	112	ALA	3.1
3	A	110	ILE	3.0
3	A	235	PHE	3.0
3	B	205	GLU	3.0
3	A	311	ALA	3.0
3	B	296	GLU	3.0
3	B	286	PHE	3.0
3	A	236	LYS	3.0
1	C	11	DG	3.0
3	B	81	CYS	3.0
3	A	35	ASN	3.0
3	A	125	ARG	3.0
3	A	42	CYS	2.9
3	B	48	ALA	2.9
3	B	127	TRP	2.9
3	B	14	PHE	2.8
1	C	1	DC	2.8
3	A	285	THR	2.8
2	D	11	DG	2.8
3	B	132	VAL	2.7
3	B	122	ASP	2.7
1	C	10	DG	2.6
2	D	22	DG	2.6
3	B	342	LEU	2.6
3	B	107	LEU	2.6
3	A	171	PRO	2.6
3	A	27	VAL	2.6
3	B	287	SER	2.6
3	B	74	GLU	2.6
2	D	10	DG	2.6
3	A	129	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
3	B	114	THR	2.6
3	B	109	PHE	2.6
3	A	278	LEU	2.5
3	A	81	CYS	2.5
3	B	277	THR	2.5
3	B	290	ASP	2.5
3	A	259	PHE	2.5
3	A	208	ASP	2.5
3	A	212	TRP	2.5
3	A	80	VAL	2.5
3	A	240	TYR	2.5
3	A	365	LYS	2.5
1	C	22	DG	2.4
3	B	185	THR	2.4
3	A	89	LEU	2.4
3	B	288	LEU	2.4
3	A	186	MET	2.4
3	B	183	ILE	2.4
3	B	212	TRP	2.4
3	A	173	PRO	2.4
3	A	231	LEU	2.3
3	B	186	MET	2.3
3	A	239	PHE	2.3
3	A	238	THR	2.3
3	A	126	GLU	2.3
3	A	118	GLN	2.3
3	A	38	ALA	2.3
3	B	207	ILE	2.3
3	A	116	ALA	2.3
3	A	29	SER	2.2
3	A	310	ASP	2.2
3	A	99	PHE	2.2
3	A	233	ASN	2.2
3	B	233	ASN	2.2
3	B	357	ALA	2.2
2	D	21	DC	2.2
3	B	359	MET	2.1
3	B	73	ASN	2.1
3	A	232	SER	2.1
3	A	295	SER	2.1
3	A	241	GLN	2.1
3	B	116	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
3	B	311	ALA	2.1
3	B	236	LYS	2.1
3	B	320	LEU	2.1
3	A	107	LEU	2.0
3	B	258	GLY	2.0
3	B	269	TRP	2.0
3	A	294	ASP	2.0
3	B	16	ALA	2.0
3	A	360	LEU	2.0
3	A	23	VAL	2.0
3	A	26	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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. 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	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	CA	B	803	1/1	0.63	0.25	115,115,115,115	0
5	CA	A	801	1/1	0.65	0.26	103,103,103,103	0
5	CA	A	802	1/1	0.86	0.37	97,97,97,97	0
4	FE	B	902	1/1	0.88	0.20	64,64,64,64	0
4	FE	A	901	1/1	0.92	0.21	64,64,64,64	0
5	CA	B	804	1/1	0.96	0.33	89,89,89,89	0

6.5 Other polymers [i](#)

There are no such residues in this entry.