



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:45 AM GMT

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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

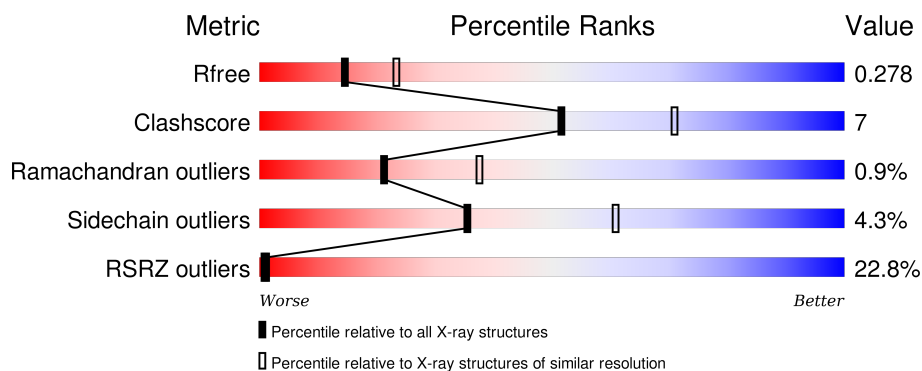
1 Overall quality at a glance

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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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. 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	<div> <div>18%</div> <div>64%</div> <div>36%</div> </div>
2	D	22	<div> <div>27%</div> <div>77%</div> <div>23%</div> </div>
3	A	383	<div> <div>21%</div> <div>77%</div> <div>13%</div> <div>8%</div> </div>
3	B	383	<div> <div>21%</div> <div>74%</div> <div>17%</div> <div>8%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CA	A	802	-	-	-	X

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*DGP*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*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 2720	C 1743	N 469	O 498	S 10	0	0	0
3	B	353	Total 2718	C 1740	N 467	O 501	S 10	0	0	0

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

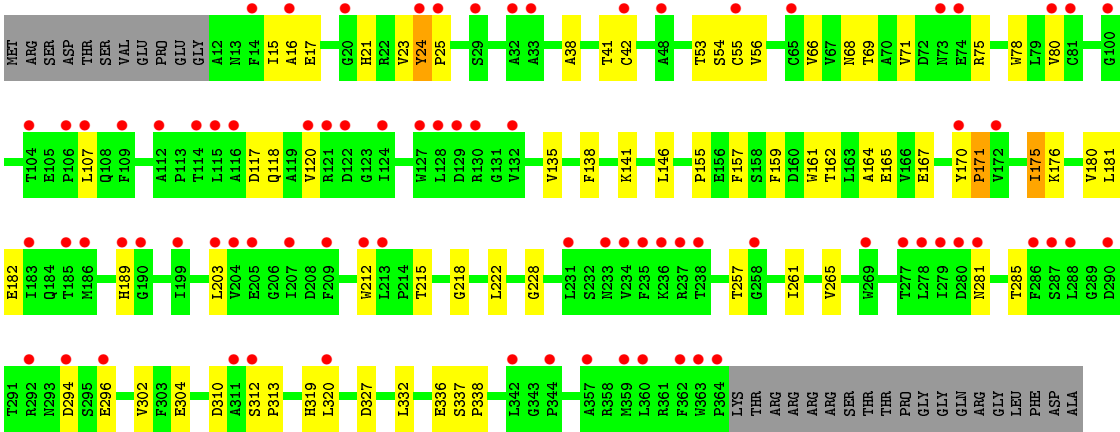
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Fe 1 1	0	0
4	A	1	Total Fe 1 1	0	0

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

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	A	56	Total O 56 56	0	0
6	B	60	Total O 60 60	0	0
6	C	25	Total O 25 25	0	0
6	D	27	Total O 27 27	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)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.223 , 0.277 0.224 , 0.278	Depositor DCC
R_{free} test set	1484 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)	0.26 , 54.3	EDS
Estimated twinning fraction	0.017 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	6 of 29457 reflections (0.020%)	Xtriage
F_o, F_c correlation	0.94	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.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Continued on next page...

Continued from previous page...

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: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

Continued on next page...

Continued from previous page...

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: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 [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%)	21	37
3	B	351/383 (92%)	328 (93%)	20 (6%)	3 (1%)	21	37
All	All	703/766 (92%)	657 (94%)	40 (6%)	6 (1%)	21	37

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%)	30	53
3	B	280/317 (88%)	270 (96%)	10 (4%)	42	69
All	All	558/634 (88%)	534 (96%)	24 (4%)	35	61

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

Continued on next page...

Continued from previous page...

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 ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

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

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%)	1.23	4 (18%) 2 2	56, 61, 72, 76	0
2	D	22/22 (100%)	1.33	6 (27%) 1 1	57, 63, 76, 78	0
3	A	354/383 (92%)	1.32	80 (22%) 1 1	26, 67, 72, 77	0
3	B	353/383 (92%)	1.40	81 (22%) 1 1	58, 67, 72, 76	0
All	All	751/810 (92%)	1.36	171 (22%) 1 1	26, 67, 72, 78	0

All (171) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	204	VAL	9.7
3	A	166	VAL	9.2
3	B	124	ILE	8.6
3	A	207	ILE	8.0
3	B	32	ALA	7.4
3	A	312	SER	7.2
3	B	199	ILE	7.2
3	A	120	VAL	7.0
3	A	284	GLY	6.7
3	A	127	TRP	6.6
3	A	172	VAL	6.6
3	A	104	THR	6.2
3	A	122	ASP	5.8
3	B	172	VAL	5.7
3	B	294	ASP	5.7
3	A	24	TYR	5.5
3	B	203	LEU	5.5
3	B	100	GLY	5.4
3	A	119	ALA	5.3
3	B	104	THR	5.2
3	B	129	ASP	5.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	B	106	PRO	5.0
3	B	115	LEU	5.0
3	A	123	GLY	5.0
3	A	132	VAL	5.0
3	A	364	PRO	5.0
3	B	213	LEU	5.0
3	A	205	GLU	5.0
3	B	170	TYR	4.8
3	B	363	TRP	4.8
3	A	65	CYS	4.8
3	B	25	PRO	4.8
3	A	169	ILE	4.7
3	B	234	VAL	4.7
3	A	282	GLY	4.6
3	B	312	SER	4.5
3	B	55	CYS	4.5
3	A	363	TRP	4.5
2	D	1	DC	4.4
3	B	281	ASN	4.3
3	B	280	ASP	4.3
3	B	128	LEU	4.2
3	B	238	THR	4.2
3	B	20	GLY	4.1
3	A	204	VAL	4.1
3	B	29	SER	4.1
3	A	283	ASP	4.0
3	A	201	ILE	4.0
3	A	293	ASN	3.9
3	A	344	PRO	3.8
3	A	55	CYS	3.8
3	B	120	VAL	3.8
3	B	279	ILE	3.8
3	B	362	PHE	3.6
3	B	364	PRO	3.6
3	B	33	ALA	3.6
3	A	134	VAL	3.6
3	B	235	PHE	3.6
3	B	121	ARG	3.6
3	B	209	PHE	3.5
3	A	345	SER	3.5
3	B	292	ARG	3.5
3	A	234	VAL	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	B	360	LEU	3.4
3	B	80	VAL	3.4
3	A	237	ARG	3.4
3	A	279	ILE	3.4
3	B	65	CYS	3.4
3	B	231	LEU	3.4
3	A	124	ILE	3.3
3	B	278	LEU	3.3
3	B	237	ARG	3.3
3	B	42	CYS	3.2
3	B	112	ALA	3.2
3	B	24	TYR	3.2
3	A	110	ILE	3.2
3	A	311	ALA	3.2
3	A	42	CYS	3.1
3	B	81	CYS	3.1
3	B	205	GLU	3.1
1	C	11	DG	3.1
3	A	235	PHE	3.1
3	B	296	GLU	3.1
3	A	236	LYS	3.1
3	B	286	PHE	3.1
3	A	35	ASN	3.1
3	A	125	ARG	3.1
3	B	48	ALA	3.1
3	B	127	TRP	3.0
3	B	14	PHE	2.9
3	A	285	THR	2.9
2	D	11	DG	2.9
3	B	132	VAL	2.9
3	B	122	ASP	2.9
1	C	1	DC	2.8
1	C	10	DG	2.8
2	D	22	DG	2.8
3	A	27	VAL	2.8
3	A	171	PRO	2.8
3	B	107	LEU	2.8
3	B	342	LEU	2.8
2	D	10	DG	2.7
3	B	114	THR	2.7
3	A	129	ASP	2.7
3	B	287	SER	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	B	74	GLU	2.7
3	A	81	CYS	2.7
3	A	278	LEU	2.7
3	B	109	PHE	2.7
3	B	290	ASP	2.7
3	B	277	THR	2.7
3	A	208	ASP	2.6
3	A	80	VAL	2.6
3	A	259	PHE	2.6
3	A	212	TRP	2.6
3	A	240	TYR	2.6
1	C	22	DG	2.6
3	A	365	LYS	2.6
3	B	185	THR	2.6
3	A	186	MET	2.6
3	B	288	LEU	2.5
3	B	183	ILE	2.5
3	A	173	PRO	2.5
3	A	89	LEU	2.5
3	B	212	TRP	2.5
3	B	186	MET	2.5
3	A	231	LEU	2.4
3	A	238	THR	2.4
3	A	239	PHE	2.4
3	A	38	ALA	2.4
3	A	126	GLU	2.4
3	A	118	GLN	2.4
3	A	116	ALA	2.4
3	B	207	ILE	2.4
3	A	310	ASP	2.4
3	A	29	SER	2.3
3	A	233	ASN	2.3
3	A	99	PHE	2.3
3	B	357	ALA	2.3
3	B	359	MET	2.3
3	B	233	ASN	2.3
3	B	73	ASN	2.3
3	B	116	ALA	2.2
3	A	241	GLN	2.2
3	A	232	SER	2.2
3	A	295	SER	2.2
3	B	311	ALA	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	21	DC	2.2
3	B	236	LYS	2.2
3	B	258	GLY	2.2
3	B	320	LEU	2.2
3	A	294	ASP	2.2
3	B	16	ALA	2.2
3	A	107	LEU	2.2
3	A	23	VAL	2.1
3	A	360	LEU	2.1
3	B	269	TRP	2.1
3	A	300	ILE	2.1
3	B	344	PRO	2.1
3	A	26	GLU	2.1
3	A	106	PRO	2.1
3	A	252	GLN	2.1
3	B	130	ARG	2.1
3	A	247	ALA	2.1
3	A	209	PHE	2.1
3	A	108	GLN	2.0
3	B	189	HIS	2.0
3	B	190	GLY	2.0
2	D	9	DC	2.0
3	A	184	GLN	2.0
3	A	131	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 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. 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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	CA	A	802	1/1	0.86	0.37	2.20	97,97,97,97	0
5	CA	B	804	1/1	0.96	0.33	0.71	89,89,89,89	0
5	CA	A	801	1/1	0.65	0.26	0.20	103,103,103,103	0
4	FE	A	901	1/1	0.92	0.21	-1.81	64,64,64,64	0
4	FE	B	902	1/1	0.88	0.20	-2.04	64,64,64,64	0
5	CA	B	803	1/1	0.63	0.25	-	115,115,115,115	0

6.5 Other polymers [i](#)

There are no such residues in this entry.