



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:07 PM UTC

PDB ID : 3C25 / pdb_00003c25
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 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

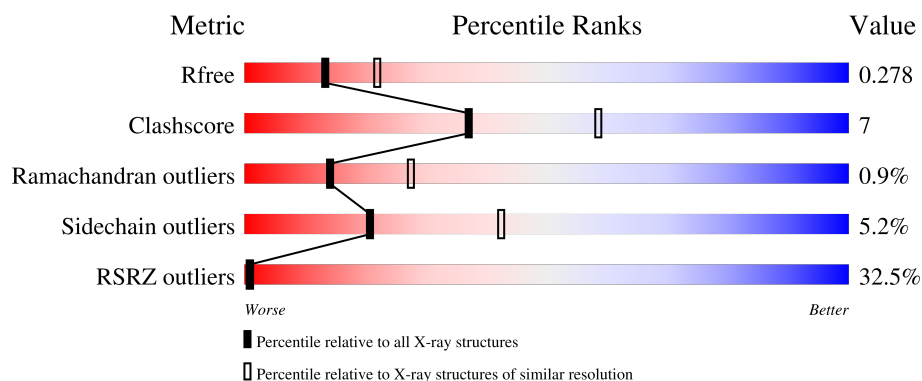
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 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	22	
2	D	22	
3	A	383	
3	B	383	

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 446	C 209	N 85	O 131	P 21	0	0	0

- 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 (CCD ID: FE) (formula: Fe).

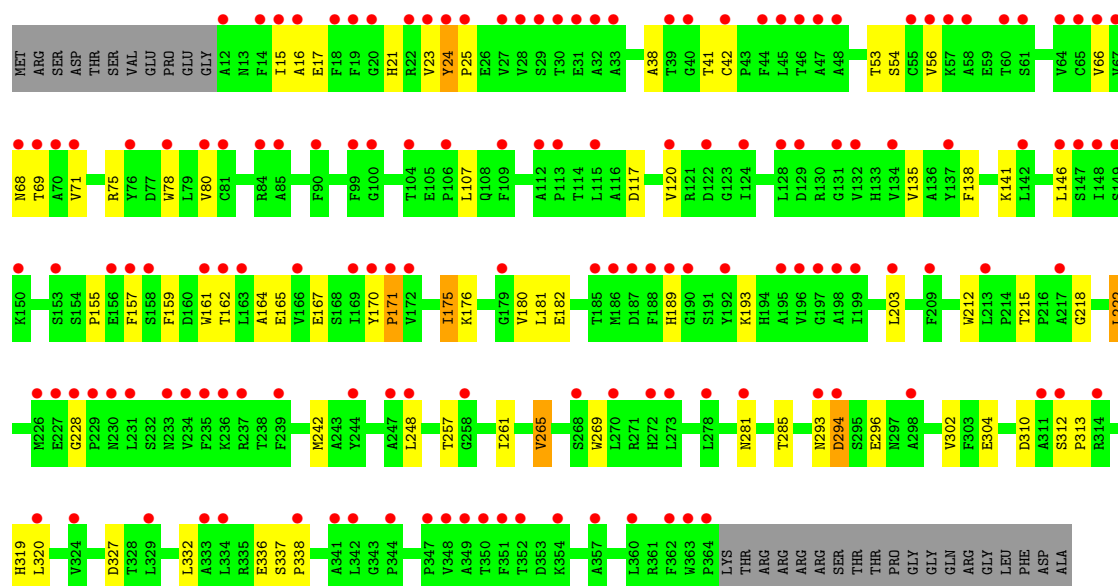
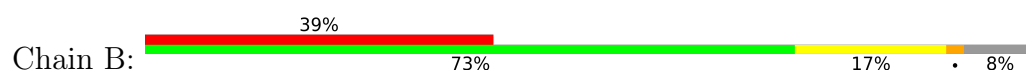
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Fe 1 1	0	0
4	B	1	Total Fe 1 1	0	0

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 6 is water.

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



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 50.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.7 (50.00-2.50) 97.7 (50.00-2.50)	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	1488 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	55.3	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 61.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for l,-k,h	Xtriage
F_o, F_c correlation	0.89	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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.22	0/505	0.93	3/778 (0.4%)
2	D	0.23	0/499	0.75	0/768
3	A	0.48	0/2795	0.79	2/3812 (0.1%)
3	B	0.48	0/2793	0.80	0/3809
All	All	0.45	0/6592	0.80	5/9167 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1	DC	O3'-P-O5'	-14.24	82.64	104.00
1	C	1	DC	OP2-P-O3'	-6.83	87.51	108.00
1	C	1	DC	OP1-P-O3'	-6.71	87.86	108.00
3	A	343	GLY	CA-C-N	5.44	125.09	119.05
3	A	343	GLY	C-N-CA	5.44	125.09	119.05

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	C	450	0	244	3	0
2	D	446	0	245	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	2720	0	2615	43	0
3	B	2718	0	2614	41	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	86	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 (86) 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	1.10
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:HG12	3:A:27:VAL:O	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	0.64
3:A:283:ASP:CG	3:A:285:THR:CG2	2.64	0.64
3:A:212:TRP:O	3:A:215:THR:HG22	1.97	0.64
1:C:8:DG:N7	3:A:189:HIS:HE1	1.99	0.60
3:A:283:ASP:OD2	3:A:285:THR:HG22	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:24:TYR:HB3	3:B:25:PRO:HD3	1.86	0.58
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:242:MET:HE1	3:B:269:TRP:HZ3	1.77	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
3:A:38:ALA:HA	3:A:203:LEU:HD21	1.99	0.44
3:A:215:THR:OG1	3:A:216:PRO:HD2	2.17	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:CG1	3:A:80:VAL:O	2.64	0.44
3:B:293:ASN:O	3:B:294:ASP:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:A:242:MET:HE1	3:A:269:TRP:HZ3	1.83	0.42
1:C:18:DC:H2"	1:C:19:DG:C8	2.54	0.42
3:B:38:ALA:HA	3:B:203:LEU:HD21	2.01	0.42
3:B:155:PRO:HG2	3:B:157:PHE:CE2	2.55	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:17:GLU:HB2	3:B:21:HIS:C	2.45	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%)	14	27
3	B	351/383 (92%)	328 (93%)	20 (6%)	3 (1%)	14	27
All	All	703/766 (92%)	657 (94%)	40 (6%)	6 (1%)	14	27

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%)	261 (94%)	17 (6%)	17	35
3	B	280/317 (88%)	268 (96%)	12 (4%)	26	51
All	All	558/634 (88%)	529 (95%)	29 (5%)	21	42

All (29) 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	74	GLU
3	A	75	ARG
3	A	79	LEU
3	A	80	VAL
3	A	97	LYS
3	A	110	ILE
3	A	114	THR
3	A	151	THR
3	A	177	ARG
3	A	193	LYS
3	A	207	ILE
3	A	234	VAL
3	A	287	SER

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Mol	Chain	Res	Type
3	B	42	CYS
3	B	71	VAL
3	B	75	ARG
3	B	107	LEU
3	B	175	ILE
3	B	193	LYS
3	B	222	LEU
3	B	248	LEU
3	B	265	VAL
3	B	296	GLU
3	B	310	ASP
3	B	327	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

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

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 oligosaccharides 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 [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	22/22 (100%)	0.88	0 100 100	56, 61, 72, 76	0
2	D	22/22 (100%)	0.90	1 (4%) 38 33	57, 63, 76, 78	0
3	A	354/383 (92%)	1.54	95 (26%) 1 1	26, 67, 72, 77	0
3	B	353/383 (92%)	1.96	148 (41%) 0 0	58, 67, 72, 76	0
All	All	751/810 (92%)	1.70	244 (32%) 1 1	26, 67, 72, 78	0

All (244) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	189	HIS	6.4
3	B	190	GLY	6.3
3	A	312	SER	5.6
3	B	55	CYS	5.5
3	B	42	CYS	5.5
3	B	65	CYS	5.3
3	B	80	VAL	5.3
3	B	228	GLY	5.2
3	B	192	TYR	4.8
3	A	42	CYS	4.7
3	B	312	SER	4.5
3	A	189	HIS	4.5
3	A	228	GLY	4.3
3	B	188	PHE	4.3
3	A	65	CYS	4.2
3	B	67	VAL	4.2
3	B	20	GLY	4.2
3	A	149	SER	4.2
3	B	81	CYS	4.2
3	B	129	ASP	4.0
3	B	115	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
3	B	16	ALA	3.9
3	A	349	ALA	3.9
3	B	334	LEU	3.8
3	B	186	MET	3.8
3	B	363	TRP	3.8
3	B	85	ALA	3.8
3	B	185	THR	3.8
3	B	237	ARG	3.8
3	B	196	VAL	3.7
3	B	69	THR	3.7
3	A	295	SER	3.7
3	B	362	PHE	3.6
3	B	61	SER	3.6
3	A	55	CYS	3.6
3	A	324	VAL	3.5
3	B	134	VAL	3.5
3	A	190	GLY	3.5
3	B	137	TYR	3.5
3	A	362	PHE	3.5
3	B	76	TYR	3.4
3	B	298	ALA	3.4
3	B	349	ALA	3.4
3	B	187	ASP	3.4
3	B	230	ASN	3.4
3	B	28	VAL	3.4
3	B	48	ALA	3.3
3	B	29	SER	3.3
3	B	172	VAL	3.3
3	B	15	ILE	3.3
3	B	33	ALA	3.3
3	B	147	SER	3.3
3	A	172	VAL	3.3
3	B	170	TYR	3.3
3	A	81	CYS	3.3
3	A	64	VAL	3.3
3	B	146	LEU	3.2
3	B	364	PRO	3.2
3	B	156	GLU	3.2
3	A	80	VAL	3.2
3	B	57	LYS	3.2
3	B	12	ALA	3.2
3	A	363	TRP	3.2

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Mol	Chain	Res	Type	RSRZ
3	A	23	VAL	3.2
3	B	124	ILE	3.2
3	B	47	ALA	3.1
3	B	324	VAL	3.1
3	B	195	ALA	3.1
3	B	247	ALA	3.1
3	B	19	PHE	3.1
3	A	127	TRP	3.1
3	B	70	ALA	3.1
3	B	45	LEU	3.1
3	B	64	VAL	3.1
3	A	364	PRO	3.1
3	B	66	VAL	3.1
3	B	14	PHE	3.0
3	A	348	VAL	3.0
3	B	169	ILE	3.0
3	B	217	ALA	3.0
3	B	171	PRO	3.0
3	A	120	VAL	3.0
3	B	148	ILE	2.9
3	B	78	TRP	2.9
3	B	294	ASP	2.9
3	B	23	VAL	2.9
3	B	227	GLU	2.9
3	A	188	PHE	2.9
3	A	290	ASP	2.9
3	B	109	PHE	2.9
3	B	46	THR	2.9
3	B	231	LEU	2.9
3	A	24	TYR	2.9
3	B	226	MET	2.9
3	B	120	VAL	2.8
3	B	347	PRO	2.8
3	B	112	ALA	2.8
3	A	52	GLU	2.8
3	A	351	PHE	2.8
3	B	149	SER	2.8
3	B	293	ASN	2.8
3	B	344	PRO	2.8
3	B	60	THR	2.8
3	A	294	ASP	2.8
3	B	157	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
3	B	209	PHE	2.8
3	B	351	PHE	2.8
3	A	230	ASN	2.8
3	A	236	LYS	2.8
3	B	106	PRO	2.7
3	B	229	PRO	2.7
3	A	119	ALA	2.7
3	A	285	THR	2.7
3	B	166	VAL	2.7
3	A	123	GLY	2.7
3	B	24	TYR	2.7
3	A	237	ARG	2.7
3	B	233	ASN	2.7
3	B	248	LEU	2.7
3	B	360	LEU	2.7
3	A	104	THR	2.7
3	B	32	ALA	2.7
3	A	301	PHE	2.6
3	B	18	PHE	2.6
3	A	233	ASN	2.6
3	B	71	VAL	2.6
3	B	348	VAL	2.6
3	A	12	ALA	2.6
3	B	333	ALA	2.6
3	A	86	LEU	2.6
3	B	27	VAL	2.6
3	A	147	SER	2.6
3	B	161	TRP	2.6
3	B	40	GLY	2.6
3	B	131	GLY	2.6
3	B	320	LEU	2.6
3	B	342	LEU	2.6
3	A	67	VAL	2.6
3	B	213	LEU	2.5
3	A	287	SER	2.5
3	B	179	GLY	2.5
3	B	31	GLU	2.5
3	A	166	VAL	2.5
3	B	163	LEU	2.5
3	B	162	THR	2.5
3	B	142	LEU	2.5
3	B	236	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
3	B	44	PHE	2.5
3	B	39	THR	2.5
3	A	99	PHE	2.4
3	A	292	ARG	2.4
3	A	352	THR	2.4
3	B	352	THR	2.4
3	A	146	LEU	2.4
3	A	227	GLU	2.4
3	B	158	SER	2.4
3	B	314	ARG	2.4
3	B	68	ASN	2.4
3	A	187	ASP	2.4
3	A	231	LEU	2.4
3	B	90	PHE	2.4
3	A	35	ASN	2.4
3	A	113	PRO	2.3
3	B	113	PRO	2.3
3	A	284	GLY	2.3
3	A	148	ILE	2.3
3	B	84	ARG	2.3
3	B	278	LEU	2.3
3	B	234	VAL	2.3
3	B	128	LEU	2.3
3	A	159	PHE	2.3
3	A	326	VAL	2.3
3	B	25	PRO	2.3
3	A	185	THR	2.3
3	B	350	THR	2.3
3	B	100	GLY	2.3
3	B	153	SER	2.3
3	A	365	LYS	2.3
3	B	239	PHE	2.3
3	B	198	ALA	2.3
3	B	281	ASN	2.3
3	A	256	GLY	2.3
3	A	261	ILE	2.3
3	A	347	PRO	2.3
3	A	192	TYR	2.3
3	A	29	SER	2.2
3	A	124	ILE	2.2
3	A	334	LEU	2.2
3	B	150	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
3	B	329	LEU	2.2
3	B	235	PHE	2.2
3	A	132	VAL	2.2
3	A	234	VAL	2.2
3	A	251	HIS	2.2
3	B	197	GLY	2.2
3	A	300	ILE	2.2
3	B	58	ALA	2.2
3	A	320	LEU	2.2
3	B	203	LEU	2.2
3	B	270	LEU	2.2
3	B	199	ILE	2.2
3	A	33	ALA	2.2
3	B	272	HIS	2.2
3	B	357	ALA	2.2
3	A	186	MET	2.2
3	A	15	ILE	2.2
3	B	56	VAL	2.1
3	B	341	ALA	2.1
3	B	258	GLY	2.1
3	B	244	TYR	2.1
3	A	246	PHE	2.1
3	B	99	PHE	2.1
3	A	293	ASN	2.1
3	A	46	THR	2.1
3	A	69	THR	2.1
3	A	76	TYR	2.1
3	B	338	PRO	2.1
3	A	71	VAL	2.1
3	A	116	ALA	2.1
3	A	217	ALA	2.1
3	B	273	LEU	2.1
3	A	358	ARG	2.1
3	A	330	ILE	2.1
3	A	240	TYR	2.1
3	A	57	LYS	2.1
3	A	129	ASP	2.1
3	A	174	LYS	2.1
3	B	354	LYS	2.1
3	A	333	ALA	2.1
3	B	311	ALA	2.1
3	B	22	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
3	B	104	THR	2.1
3	B	122	ASP	2.1
3	A	25	PRO	2.1
3	A	252	GLN	2.0
3	A	28	VAL	2.0
3	B	132	VAL	2.0
2	D	20	DC	2.0
3	B	30	THR	2.0
3	A	173	PRO	2.0
3	B	268	SER	2.0
3	A	30	THR	2.0
3	A	344	PRO	2.0
3	A	337	SER	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](#)

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	A	801	1/1	0.68	0.27	103,103,103,103	0
5	CA	B	804	1/1	0.82	0.48	89,89,89,89	0
5	CA	B	803	1/1	0.83	0.18	115,115,115,115	0
5	CA	A	802	1/1	0.86	0.23	97,97,97,97	0
4	FE	A	901	1/1	0.90	0.14	64,64,64,64	0
4	FE	B	902	1/1	0.93	0.10	64,64,64,64	0

6.5 Other polymers [i](#)

There are no such residues in this entry.