



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:40 PM UTC

PDB ID : 1EZS / pdb_00001ezs
Title : CRYSTAL STRUCTURE OF ECOTIN MUTANT M84R, W67A, G68A, Y69A, D70A BOUND TO RAT ANIONIC TRYPSIN II
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Deposited on : 2000-05-11
Resolution : 2.30 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

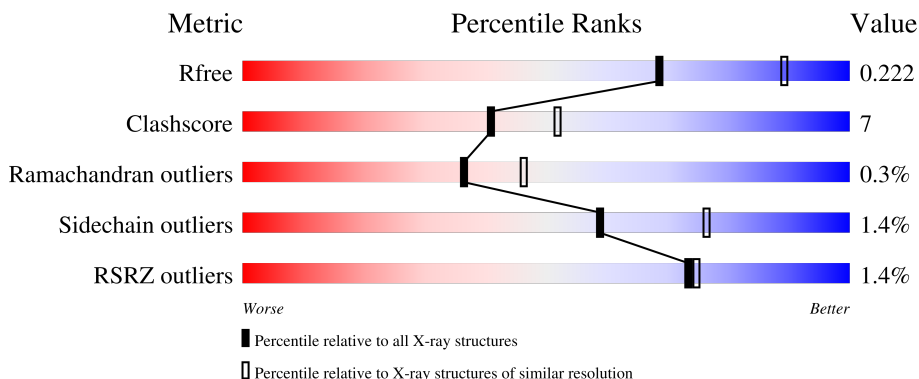
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	A	142	3% 75% 12% • 12%
1	B	142	4% 77% 9% • 12%
2	C	223	83% 16% •
2	D	223	82% 16% •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5332 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 ECOTIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	125	Total	C	N	O	S	0	0	0
			956	604	159	188	5			
1	B	125	Total	C	N	O	S	0	0	0
			956	604	159	188	5			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	ALA	TRP	engineered mutation	UNP P23827
A	68	ALA	GLY	engineered mutation	UNP P23827
A	69	ALA	TYR	engineered mutation	UNP P23827
A	70	ALA	ASP	engineered mutation	UNP P23827
A	84	ARG	MET	engineered mutation	UNP P23827
B	267	ALA	TRP	engineered mutation	UNP P23827
B	268	ALA	GLY	engineered mutation	UNP P23827
B	269	ALA	TYR	engineered mutation	UNP P23827
B	270	ALA	ASP	engineered mutation	UNP P23827
B	284	ARG	MET	engineered mutation	UNP P23827

- Molecule 2 is a protein called TRYPSIN II, ANIONIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	223	Total	C	N	O	S	0	0	0
			1666	1041	285	326	14			
2	D	223	Total	C	N	O	S	0	0	0
			1666	1041	285	326	14			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	479	ASP	ASN	SEE REMARK 999	UNP P00763
C	502	ASN	ASP	engineered mutation	UNP P00763

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Chain	Residue	Modelled	Actual	Comment	Reference
D	779	ASP	ASN	SEE REMARK 999	UNP P00763
D	802	ASN	ASP	engineered mutation	UNP P00763

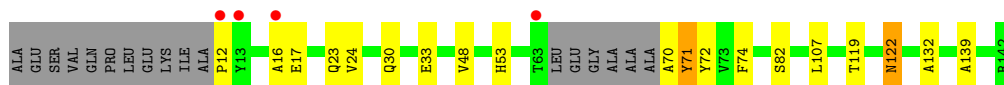
- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total Ca 1 1	0	0
3	D	1	Total Ca 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	8	Total O 8 8	0	0
4	B	6	Total O 6 6	0	0
4	C	36	Total O 36 36	0	0
4	D	36	Total O 36 36	0	0

- Molecule 1: ECOTIN



ALA
GLU
SER
VAL
GLN
PRO
LEU
GLU
GLU
LYS
ILE
ALA
P212
A216
E217
Q223
Q230
E233
V248
H253
T263
LEU
GLU
GLY
ALA
ALA
ALA
A270
V271
V272
S279
C287
L307
T319
N322
W330
V345

V613	P428	G438	S445	V453	A456	B462	H471	L476	N474	V475	Q481	K497	N502	L503	H504	K513	L514	N515	A516	H517	V518	A519	C536	G548	V549	L562	L563	T577	D578	N579	V583	S590	P598	V599	V600		
Y429	Y429	Y429	L446	L447	L447	L447	L472	L473	L474	L475	L476	L477	L478	L479	L480	L481	L482	L483	L484	L485	L486	L487	L488	L489	L490	L491	L492	L493	L494	L495	L496	L497	L498	L499	L500	L501	L502

P888	P889	L909	V913	S914	W915	Y928	V931	I945	T716	T717	S726	T727	P728	G738	S745	A756	H757	R762	H771	W772	T773	W774	V775	G781	T789	T798	L799	M802	B803	M804	K813	L814	M815	A816	B817	V818	A819	P824	C836	T844	V849	M850	E851	L862	L863	T877	D878	M879	S890
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	45.83Å 59.68Å 71.04Å 103.57° 93.27° 94.62°	Depositor
Resolution (Å)	25.00 – 2.30 25.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	92.7 (25.00-2.30) 92.8 (25.00-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 2.31Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.188 , 0.235 0.180 , 0.222	Depositor DCC
R_{free} test set	1512 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	31.5	Xtriage
Anisotropy	0.282	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5332	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.40% 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 ⓘ

5.1 Standard geometry ⓘ

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

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	A	0.81	0/972	0.95	2/1321 (0.2%)
1	B	0.77	0/972	1.00	5/1321 (0.4%)
2	C	0.77	0/1701	1.04	8/2318 (0.3%)
2	D	0.88	2/1701 (0.1%)	1.11	9/2318 (0.4%)
All	All	0.82	2/5346 (0.0%)	1.04	24/7278 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	913	VAL	CA-CB	5.96	1.61	1.54
2	D	849	VAL	CA-CB	5.23	1.60	1.54

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	789	ILE	N-CA-C	7.69	117.78	106.85
2	D	915	TRP	N-CA-C	7.57	118.59	108.38
2	D	849	VAL	N-CA-C	6.60	117.39	107.75
1	B	287	CYS	CA-C-N	6.52	126.02	119.24
1	B	287	CYS	C-N-CA	6.52	126.02	119.24
1	B	212	PRO	N-CA-CB	6.44	110.09	103.00
1	A	12	PRO	N-CA-CB	6.38	110.01	103.00
2	C	438	GLY	N-CA-C	-6.22	106.84	114.92
2	D	774	ASN	N-CA-C	6.14	120.91	113.17
2	D	738	GLY	N-CA-C	-6.13	106.95	114.92
2	C	549	VAL	N-CA-C	6.12	116.69	107.75
2	D	890	SER	N-CA-C	-5.73	103.14	110.53
2	C	497	LYS	N-CA-C	5.68	118.24	111.71
2	C	615	TRP	N-CA-C	5.38	115.64	108.38
2	D	931	VAL	N-CA-C	5.38	116.11	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	548	GLY	N-CA-C	-5.37	104.86	112.81
1	B	279	SER	CA-C-N	5.30	126.47	119.84
1	B	279	SER	C-N-CA	5.30	126.47	119.84
2	C	598	PRO	N-CA-C	5.23	119.52	111.57
2	C	474	ASN	N-CA-C	5.21	119.74	113.17
2	D	851	GLU	CA-C-N	5.14	125.34	120.31
2	D	851	GLU	C-N-CA	5.14	125.34	120.31
1	A	139	ALA	N-CA-C	-5.06	103.72	110.55
2	C	590	SER	N-CA-C	-5.00	103.45	110.35

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	A	956	0	908	10	0
1	B	956	0	908	8	0
2	C	1666	0	1603	24	0
2	D	1666	0	1603	27	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	8	0	0	0	0
4	B	6	0	0	0	0
4	C	36	0	0	3	0
4	D	36	0	0	2	0
All	All	5332	0	5022	67	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 (67) 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)
2:C:481:GLN:HE22	2:C:513:LYS:H	1.35	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:ASN:HD22	1:B:322:ASN:H	1.38	0.71
2:C:457:HIS:H	2:C:502:ASN:HD21	1.39	0.70
2:D:757:HIS:H	2:D:802:ASN:HD21	1.39	0.70
2:D:781:GLN:HE22	2:D:813:LYS:H	1.40	0.70
2:D:728:PRO:HB2	2:D:819:ALA:HB3	1.78	0.64
2:C:428:PRO:HB2	2:C:519:ALA:HB3	1.80	0.63
2:D:877:THR:HG22	2:D:878:ASP:N	2.13	0.63
1:A:122:ASN:HD22	1:A:122:ASN:H	1.48	0.60
2:D:772:ASN:HD22	2:D:774:ASN:H	1.50	0.58
2:C:456:ALA:HA	2:C:504:MET:HB2	1.86	0.57
2:D:836:CYS:SG	2:D:862:LEU:HD13	2.45	0.57
2:C:472:ASN:ND2	2:C:475:VAL:HG12	2.20	0.57
2:D:879:ASN:HB2	4:D:44:HOH:O	2.05	0.57
2:C:583:VAL:HB	2:C:628:TYR:CE1	2.40	0.56
1:A:16:ALA:O	1:A:17:GLU:HB3	2.04	0.56
1:B:216:ALA:O	1:B:217:GLU:HB3	2.07	0.55
2:C:536:CYS:SG	2:C:562:LEU:HD13	2.48	0.54
2:D:877:THR:HG22	2:D:878:ASP:H	1.71	0.54
2:C:636:ASP:HB2	4:C:69:HOH:O	2.06	0.54
2:C:577:THR:HG22	2:C:578:ASP:N	2.23	0.53
2:C:579:ASN:HB2	4:C:88:HOH:O	2.09	0.53
2:C:613:VAL:HG22	2:C:628:TYR:HE2	1.75	0.52
1:B:248:VAL:HB	1:B:253:HIS:CE1	2.45	0.52
1:B:272:TYR:OH	1:B:307:LEU:HD22	2.09	0.51
1:A:30:GLN:HB2	1:A:33:GLU:HG2	1.93	0.51
2:D:756:ALA:HA	2:D:804:MET:HB2	1.93	0.50
2:C:613:VAL:HA	2:C:628:TYR:CD2	2.47	0.49
1:A:72:TYR:OH	1:A:107:LEU:HD22	2.13	0.48
2:D:717:VAL:HG22	2:D:844:THR:C	2.38	0.48
2:C:577:THR:HG22	2:C:578:ASP:H	1.79	0.48
2:D:824:PRO:HD3	2:D:909:LEU:O	2.14	0.48
2:C:462:ARG:HA	2:C:462:ARG:NE	2.29	0.47
2:C:472:ASN:HD22	2:C:474:ASN:H	1.62	0.47
2:C:445:SER:OG	2:C:598:PRO:HB3	2.16	0.46
1:B:230:GLN:HB2	1:B:233:GLU:HG2	1.97	0.46
2:C:456:ALA:N	2:C:502:ASN:ND2	2.64	0.46
2:D:745:SER:OG	2:D:898:PRO:HB3	2.16	0.46
1:A:132:ALA:HB2	1:B:330:TRP:CE2	2.52	0.45
2:C:429:TYR:CZ	2:C:600:VAL:HG21	2.51	0.45
1:A:74:PHE:HB3	1:A:119:THR:HG22	1.98	0.44
2:C:472:ASN:CG	2:C:475:VAL:HG12	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:913:VAL:HG22	2:D:928:TYR:CE2	2.52	0.44
2:D:772:ASN:CG	2:D:775:VAL:HG12	2.42	0.44
2:C:515:ASN:OD1	2:C:517:ARG:HG2	2.17	0.43
1:A:23:GLN:NE2	1:A:119:THR:OG1	2.51	0.43
2:C:471:HIS:HD2	4:C:85:HOH:O	2.00	0.43
1:B:322:ASN:HD22	1:B:322:ASN:N	2.06	0.43
2:D:877:THR:CG2	2:D:878:ASP:N	2.81	0.43
2:C:472:ASN:ND2	2:C:474:ASN:H	2.16	0.43
2:D:899:VAL:HG21	2:D:928:TYR:CD2	2.54	0.42
2:D:913:VAL:HG22	2:D:928:TYR:HE2	1.83	0.42
2:D:798:THR:O	2:D:799:LEU:HB2	2.20	0.42
2:D:772:ASN:ND2	2:D:774:ASN:H	2.15	0.42
1:B:223:GLN:NE2	1:B:319:THR:OG1	2.52	0.42
2:D:771:HIS:HD2	4:D:41:HOH:O	2.02	0.42
2:D:928:TYR:CD1	2:D:928:TYR:N	2.87	0.42
2:C:447:ILE:HD13	2:C:453:VAL:CG2	2.49	0.41
2:C:613:VAL:HG22	2:C:628:TYR:CE2	2.53	0.41
2:D:726:SER:C	2:D:728:PRO:HD3	2.45	0.41
2:D:815:ASN:OD1	2:D:817:ARG:HG2	2.21	0.41
1:A:48:VAL:HB	1:A:53:HIS:CE1	2.54	0.41
1:A:82:SER:O	2:D:915:TRP:HB2	2.21	0.41
2:D:772:ASN:ND2	2:D:775:VAL:HG12	2.36	0.41
2:D:836:CYS:SG	2:D:862:LEU:CD1	3.09	0.41
1:A:70:ALA:O	1:A:71:TYR:HB3	2.21	0.40
2:D:762:ARG:NE	2:D:762:ARG:HA	2.36	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	A	121/142 (85%)	113 (93%)	7 (6%)	1 (1%)	16 20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	121/142 (85%)	113 (93%)	7 (6%)	1 (1%)	16	20
2	C	221/223 (99%)	212 (96%)	9 (4%)	0	100	100
2	D	221/223 (99%)	213 (96%)	8 (4%)	0	100	100
All	All	684/730 (94%)	651 (95%)	31 (4%)	2 (0%)	36	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	71	TYR
1	B	217	GLU

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	
1	A	100/122 (82%)	98 (98%)	2 (2%)	48	67
1	B	100/122 (82%)	99 (99%)	1 (1%)	68	82
2	C	185/185 (100%)	182 (98%)	3 (2%)	55	73
2	D	185/185 (100%)	183 (99%)	2 (1%)	65	81
All	All	570/614 (93%)	562 (99%)	8 (1%)	59	76

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	VAL
1	A	122	ASN
1	B	322	ASN
2	C	472	ASN
2	C	563	LEU
2	C	601	CYS
2	D	772	ASN
2	D	863	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	44	GLN
1	A	53	HIS
1	A	122	ASN
1	B	223	GLN
1	B	253	HIS
1	B	322	ASN
2	C	425	ASN
2	C	472	ASN
2	C	481	GLN
2	C	502	ASN
2	C	556	GLN
2	D	725	ASN
2	D	771	HIS
2	D	772	ASN
2	D	781	GLN
2	D	801	ASN
2	D	802	ASN
2	D	835	GLN
2	D	945	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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	A	125/142 (88%)	0.05	4 (3%) 50 52	15, 42, 73, 84	0
1	B	125/142 (88%)	0.08	5 (4%) 42 44	18, 43, 76, 85	0
2	C	223/223 (100%)	-0.10	1 (0%) 88 89	18, 37, 58, 77	0
2	D	223/223 (100%)	-0.46	0 100 100	10, 26, 50, 70	0
All	All	696/730 (95%)	-0.15	10 (1%) 73 75	10, 36, 67, 85	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	263	THR	3.0
1	B	216	ALA	2.6
1	A	63	THR	2.5
1	A	16	ALA	2.4
1	B	212	PRO	2.3
2	C	579	ASN	2.2
1	B	270	ALA	2.1
1	B	271	TYR	2.1
1	A	13	TYR	2.0
1	A	12	PRO	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($\text{\AA}^2$)	Q<0.9
3	CA	D	950	1/1	0.93	0.05	33,33,33,33	0
3	CA	C	650	1/1	0.94	0.08	55,55,55,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.