



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:59 AM UTC

PDB ID : 1K6Z / pdb_00001k6z
Title : Crystal Structure of the Yersinia Secretion Chaperone SycE
Authors : Evdokimov, A.G.; Tropea, J.E.; Routzahn, K.M.; Waugh, D.S.
Deposited on : 2001-10-17
Resolution : 2.00 Å(reported)

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

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<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
Mogul : 2022.3.0, CSD as543be (2022)
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

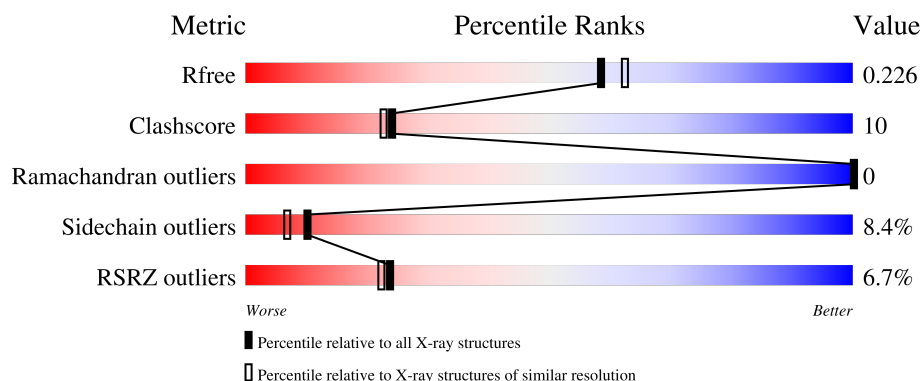
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	141	6% 69% 13% • 13%
1	B	141	6% 57% 26% • 14%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2161 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 Type III secretion chaperone SycE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	122	Total	C	N	O	S	Se	0	1	0
			983	625	168	187	1	2			
1	B	121	Total	C	N	O	S	Se	0	1	0
			974	620	166	185	1	2			

There are 28 discrepancies between the modelled and reference sequences:

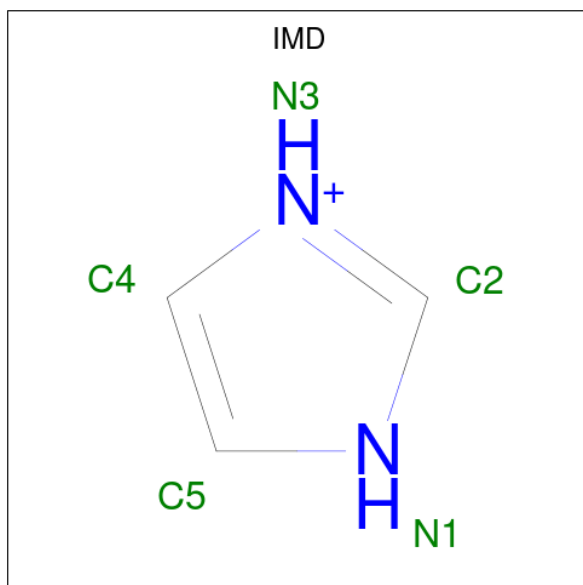
Chain	Residue	Modelled	Actual	Comment	Reference
A	996	ASP	-	expression tag	UNP P31491
A	997	TYR	-	expression tag	UNP P31491
A	998	LYS	-	expression tag	UNP P31491
A	999	ASP	-	expression tag	UNP P31491
A	1000	GLU	-	expression tag	UNP P31491
A	1001	MSE	MET	modified residue	UNP P31491
A	1048	MSE	MET	modified residue	UNP P31491
A	1109	MSE	MET	modified residue	UNP P31491
A	1131	HIS	-	expression tag	UNP P31491
A	1132	HIS	-	expression tag	UNP P31491
A	1133	HIS	-	expression tag	UNP P31491
A	1134	HIS	-	expression tag	UNP P31491
A	1135	HIS	-	expression tag	UNP P31491
A	1136	HIS	-	expression tag	UNP P31491
B	1996	ASP	-	expression tag	UNP P31491
B	1997	TYR	-	expression tag	UNP P31491
B	1998	LYS	-	expression tag	UNP P31491
B	1999	ASP	-	expression tag	UNP P31491
B	2000	GLU	-	expression tag	UNP P31491
B	2001	MSE	MET	modified residue	UNP P31491
B	2048	MSE	MET	modified residue	UNP P31491
B	2109	MSE	MET	modified residue	UNP P31491
B	2131	HIS	-	expression tag	UNP P31491
B	2132	HIS	-	expression tag	UNP P31491
B	2133	HIS	-	expression tag	UNP P31491

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Chain	Residue	Modelled	Actual	Comment	Reference
B	2134	HIS	-	expression tag	UNP P31491
B	2135	HIS	-	expression tag	UNP P31491
B	2136	HIS	-	expression tag	UNP P31491

- Molecule 2 is IMIDAZOLE (CCD ID: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			5	3	2		
2	B	1	Total	C	N	0	0
			5	3	2		

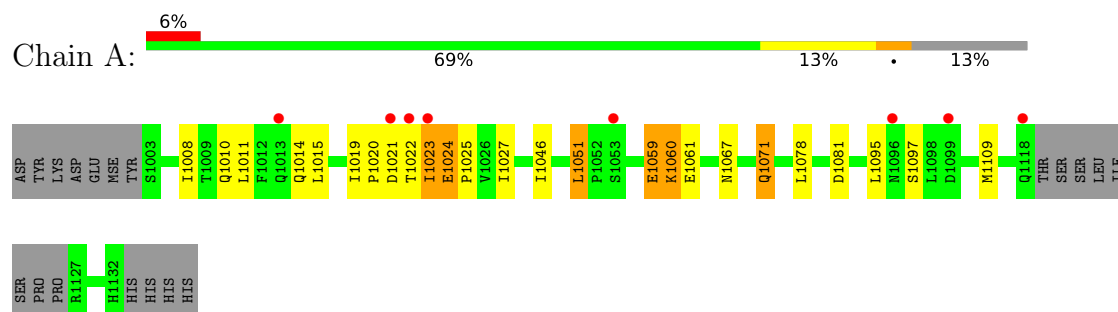
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	100	Total	O	0	0
			100	100		
3	B	94	Total	O	0	0
			94	94		

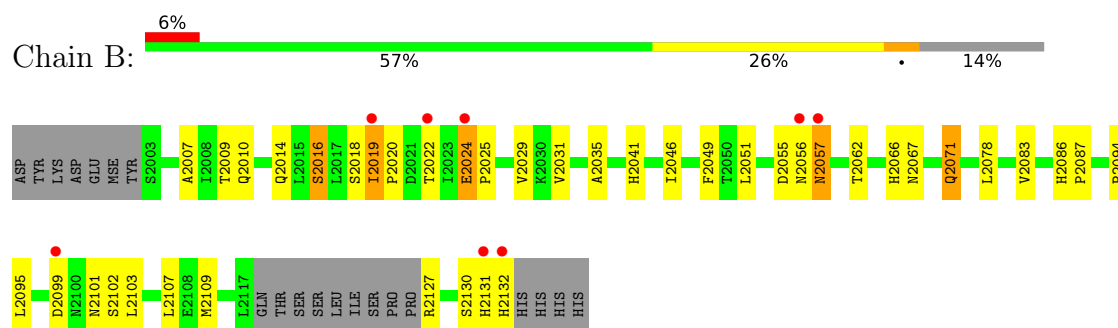
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Type III secretion chaperone SycE



- Molecule 1: Type III secretion chaperone SycE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.88Å 56.04Å 54.99Å 90.00° 114.04° 90.00°	Depositor
Resolution (Å)	35.00 – 2.00 35.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (35.00-2.00) 95.5 (35.00-2.00)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.53 (at 2.00Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.194 , 0.248 0.197 , 0.226	Depositor DCC
R_{free} test set	1062 reflections (5.38%)	wwPDB-VP
Wilson B-factor (Å ²)	22.2	Xtriage
Anisotropy	0.319	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 74.8	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	0.94	EDS
Total number of atoms	2161	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.21% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.49	1/1007 (0.1%)	1.27	4/1365 (0.3%)
1	B	0.51	0/998	1.34	4/1353 (0.3%)
All	All	0.50	1/2005 (0.0%)	1.31	8/2718 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1109	MSE	SE-CE	-5.07	1.80	1.95

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2057	ASN	CA-CB-CG	6.62	119.22	112.60
1	A	1081	ASP	CA-C-N	6.39	128.84	120.28
1	A	1081	ASP	C-N-CA	6.39	128.84	120.28
1	A	1071	GLN	CA-C-N	-5.61	115.55	122.84
1	A	1071	GLN	C-N-CA	-5.61	115.55	122.84
1	B	2055	ASP	O-C-N	5.58	129.54	123.13
1	B	2049	PHE	CA-CB-CG	5.19	118.99	113.80
1	B	2094	PRO	CB-CA-C	-5.04	105.29	111.64

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	A	983	0	961	16	0
1	B	974	0	953	24	0
2	A	5	0	5	0	0
2	B	5	0	5	1	0
3	A	100	0	0	1	0
3	B	94	0	0	3	0
All	All	2161	0	1924	39	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 10.

All (39) 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)
1:A:1067:ASN:HD21	1:A:1078:LEU:H	1.05	1.00
1:B:2009:THR:HA	1:B:2019:ILE:HD11	1.48	0.92
1:B:2067:ASN:HD21	1:B:2078:LEU:H	1.23	0.83
1:B:2046:ILE:HD11	1:B:2095:LEU:HD13	1.68	0.76
1:B:2010:GLN:O	1:B:2014:GLN:HG3	1.86	0.74
1:A:1067:ASN:ND2	1:A:1078:LEU:H	1.84	0.74
1:A:1010:GLN:O	1:A:1014:GLN:HG3	1.90	0.71
1:A:1046:ILE:HD11	1:A:1095:LEU:HD13	1.71	0.71
1:A:1051:LEU:HB3	3:A:3025:HOH:O	1.92	0.68
1:A:1008:ILE:HG21	1:A:1027:ILE:HD13	1.77	0.66
1:B:2035:ALA:HB1	1:B:2132:HIS:CE1	2.37	0.59
1:B:2031:VAL:CG1	1:B:2127:ARG:HD2	2.33	0.58
1:B:2067:ASN:ND2	1:B:2078:LEU:H	1.99	0.57
1:B:2083:VAL:O	2:B:2502:IMD:H2	2.04	0.56
1:A:1060:LYS:HG2	1:A:1061:GLU:N	2.22	0.55
1:A:1071:GLN:HG2	1:B:2041:HIS:CE1	2.43	0.53
1:A:1059:GLU:OE2	1:A:1059:GLU:HA	2.07	0.53
1:B:2020:PRO:HD3	1:B:2131:HIS:NE2	2.26	0.50
1:A:1024:GLU:HA	1:A:1024:GLU:OE1	2.12	0.50
1:B:2101:ASN:HD22	1:B:2101:ASN:N	2.09	0.50
1:B:2046:ILE:CD1	1:B:2095:LEU:HD13	2.40	0.49
1:B:2016:SER:O	1:B:2016:SER:OG	2.31	0.47
1:B:2019:ILE:HG22	1:B:2019:ILE:O	2.14	0.47
1:A:1011:LEU:O	1:A:1015:LEU:HG	2.15	0.46
1:B:2014:GLN:NE2	3:B:3075:HOH:O	2.50	0.45
1:B:2099:ASP:OD1	1:B:2102:SER:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1023:ILE:HG22	1:A:1023:ILE:O	2.18	0.44
1:B:2007:ALA:HB1	1:B:2103:LEU:HD11	2.00	0.43
1:B:2086:HIS:HB2	1:B:2087:PRO:HD2	2.01	0.43
1:B:2071:GLN:HE21	1:B:2071:GLN:HB2	1.58	0.42
1:B:2024:GLU:CD	1:B:2025:PRO:HD2	2.45	0.42
1:B:2066:HIS:HE1	3:B:3020:HOH:O	2.02	0.42
1:A:1059:GLU:OE1	1:A:1060:LYS:HD2	2.20	0.42
1:B:2062:THR:HG23	3:B:3158:HOH:O	2.21	0.41
1:A:1019:ILE:HA	1:A:1020:PRO:HD3	1.69	0.41
1:A:1059:GLU:CD	1:A:1060:LYS:H	2.29	0.41
1:B:2029:VAL:CA	1:B:2132:HIS:HB3	2.52	0.40
1:B:2109:MSE:HA	1:B:2109:MSE:HE2	2.04	0.40
1:A:1024:GLU:HB3	1:A:1025:PRO:HD2	2.04	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	
1	A	119/141 (84%)	115 (97%)	4 (3%)	0	100	100
1	B	118/141 (84%)	117 (99%)	1 (1%)	0	100	100
All	All	237/282 (84%)	232 (98%)	5 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	
1	A	114/129 (88%)	106 (93%)	8 (7%)	14	10
1	B	113/129 (88%)	102 (90%)	11 (10%)	8	5
All	All	227/258 (88%)	208 (92%)	19 (8%)	10	7

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1021	ASP
1	A	1022	THR
1	A	1023	ILE
1	A	1024	GLU
1	A	1051	LEU
1	A	1059	GLU
1	A	1060	LYS
1	A	1097	SER
1	B	2016	SER
1	B	2018	SER
1	B	2019	ILE
1	B	2022	THR
1	B	2024	GLU
1	B	2051	LEU
1	B	2056	ASN
1	B	2057	ASN
1	B	2071	GLN
1	B	2107	LEU
1	B	2130	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1013	GLN
1	A	1066	HIS
1	A	1067	ASN
1	A	1112	GLN
1	B	2010	GLN
1	B	2014	GLN
1	B	2041	HIS
1	B	2066	HIS

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Mol	Chain	Res	Type
1	B	2067	ASN
1	B	2071	GLN
1	B	2100	ASN
1	B	2101	ASN
1	B	2132	HIS

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](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	IMD	A	2501	-	5,5,5	0.73	0	5,5,5	0.93	0
2	IMD	B	2502	-	5,5,5	0.73	0	5,5,5	0.66	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	IMD	A	2501	-	-	-	0/1/1/1
2	IMD	B	2502	-	-	-	0/1/1/1

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2502	IMD	1	0

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 [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	120/141 (85%)	0.19	8 (6%) 24 22	8, 24, 55, 88	1 (0%)
1	B	119/141 (84%)	0.13	8 (6%) 24 22	8, 24, 55, 88	1 (0%)
All	All	239/282 (84%)	0.16	16 (6%) 24 22	8, 24, 55, 88	2 (0%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1023	ILE	3.8
1	B	2132	HIS	3.8
1	B	2022	THR	3.5
1	B	2131	HIS	3.3
1	B	2057	ASN	3.3
1	B	2019	ILE	3.2
1	A	1053	SER	3.1
1	A	1022	THR	2.9
1	A	1096	ASN	2.8
1	A	1099	ASP	2.4
1	A	1118	GLN	2.4
1	B	2099	ASP	2.3
1	B	2024	GLU	2.2
1	B	2056	ASN	2.1
1	A	1013	GLN	2.0
1	A	1021	ASP	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
2	IMD	B	2502	5/5	0.88	0.22	75,75,77,77	0
2	IMD	A	2501	5/5	0.96	0.06	9,15,21,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.