



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:04 AM UTC

PDB ID : 5ISZ / pdb_00005isz
Title : Crystal structure of LS01-TCR/M1-HLA-A*02 complex
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Deposited on : 2016-03-15
Resolution : 2.06 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
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

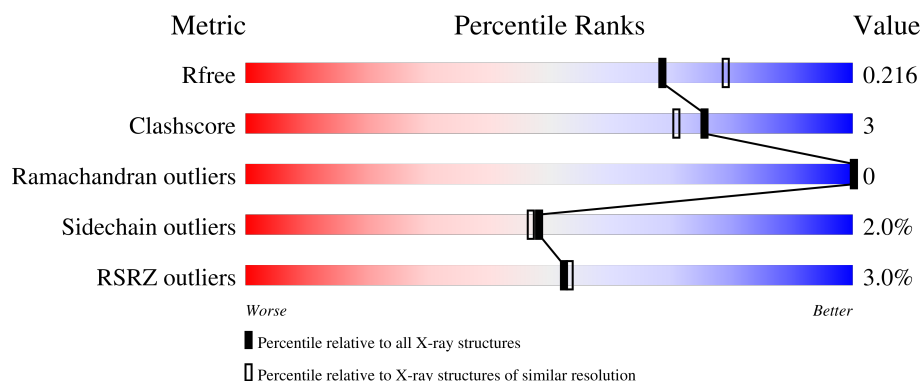
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.06 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	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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	275	6% 94% 6%
2	B	98	96% ..
3	C	9	89% 11%
4	D	200	6% 92% 6% .
5	E	241	4% 93% 6%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13509 atoms, of which 6265 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 HLA class I histocompatibility antigen, A-2 alpha chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	275	Total	C	H	N	O	S	0	0	0
			4340	1403	2094	409	425	9			

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	98	Total	C	H	N	O	S	0	0	0
			1602	522	781	139	157	3			

- Molecule 3 is a protein called influenza M1 for peptide.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	9	Total	C	H	N	O		0	0	0
			144	49	75	9	11				

- Molecule 4 is a protein called TCRalpha chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	200	Total	C	H	N	O	S	0	2	0
			3039	985	1470	256	320	8			

- Molecule 5 is a protein called TCRbeta chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
5	E	241	Total	C	H	N	O	S	0	0	0
			3739	1216	1821	334	362	6			

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			14	3	8	3		
6	A	1	Total	C	H	O	0	0
			14	3	8	3		
6	B	1	Total	C	H	O	0	0
			14	3	8	3		

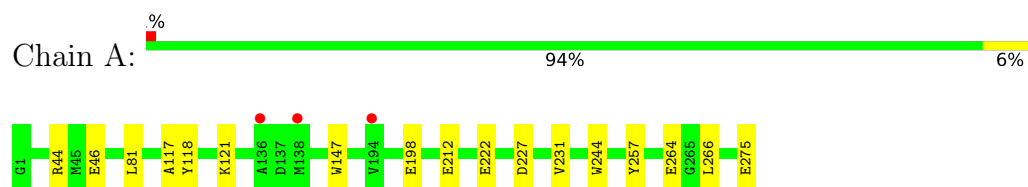
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	229	Total	O	0	0
			229	229		
7	B	99	Total	O	0	0
			99	99		
7	C	6	Total	O	0	0
			6	6		
7	D	136	Total	O	0	0
			136	136		
7	E	133	Total	O	0	0
			133	133		

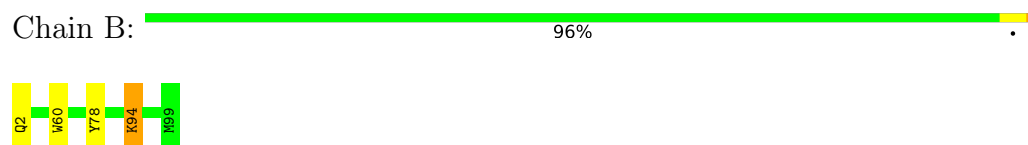
3 Residue-property plots [i](#)

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.

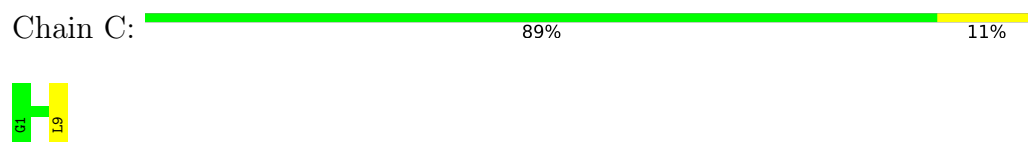
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



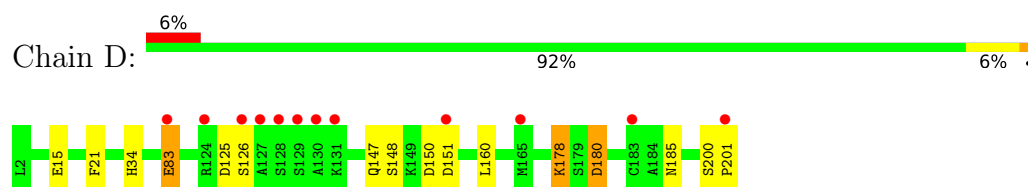
- Molecule 2: Beta-2-microglobulin



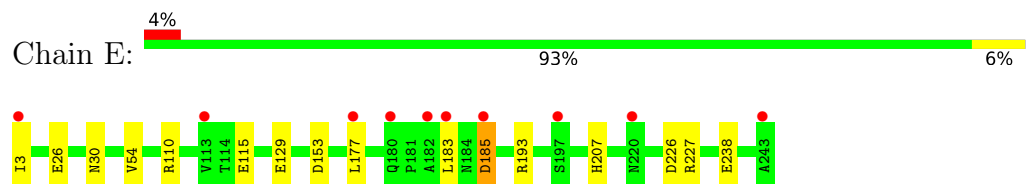
- Molecule 3: influenza M1 for peptide



- Molecule 4: TCRalpha chain



- Molecule 5: TCRbeta chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.81Å 75.46Å 121.20Å 90.00° 98.01° 90.00°	Depositor
Resolution (Å)	29.14 – 2.06 29.14 – 2.06	Depositor EDS
% Data completeness (in resolution range)	80.5 (29.14-2.06) 79.1 (29.14-2.06)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.18	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.94 (at 2.06Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.184 , 0.200 (Not available) , 0.216	Depositor DCC
R_{free} test set	2842 reflections (4.02%)	wwPDB-VP
Wilson B-factor (Å ²)	25.5	Xtriage
Anisotropy	0.500	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 46.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13509	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% 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: GOL

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	0.23	0/2311	0.41	0/3137
2	B	0.22	0/844	0.40	0/1141
3	C	0.31	0/70	0.38	0/92
4	D	0.22	0/1610	0.41	0/2187
5	E	0.21	0/1971	0.37	0/2683
All	All	0.22	0/6806	0.40	0/9240

There are no bond length outliers.

There are no bond angle outliers.

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	2246	2094	2096	15	0
2	B	821	781	780	4	0
3	C	69	75	75	2	0
4	D	1569	1470	1470	11	0
5	E	1918	1821	1821	10	0
6	A	12	16	16	1	0
6	B	6	8	8	0	0
7	A	229	0	0	9	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	99	0	0	3	1
7	C	6	0	0	0	0
7	D	136	0	0	5	2
7	E	133	0	0	6	0
All	All	7244	6265	6266	39	3

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 3.

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)
4:D:83:GLU:OE2	7:D:301:HOH:O	1.79	0.98
2:B:2:GLN:N	7:B:301:HOH:O	1.99	0.94
1:A:264:GLU:OE2	7:A:401:HOH:O	1.99	0.80
1:A:266:LEU:O	7:A:402:HOH:O	2.01	0.79
1:A:275:GLU:OE1	7:A:403:HOH:O	2.02	0.77
1:A:46:GLU:OE2	7:A:404:HOH:O	2.03	0.76
4:D:147:GLN:OE1	7:D:302:HOH:O	2.03	0.75
4:D:125:ASP:OD1	4:D:126:SER:N	2.29	0.66
5:E:227:ARG:O	7:E:302:HOH:O	2.12	0.66
1:A:222:GLU:OE1	7:A:406:HOH:O	2.12	0.65
1:A:257:TYR:O	7:A:405:HOH:O	2.12	0.65
5:E:110:ARG:NH2	5:E:153:ASP:OD2	2.31	0.63
1:A:44:ARG:NH1	6:A:302:GOL:O2	2.32	0.62
1:A:227:ASP:O	7:A:407:HOH:O	2.16	0.59
4:D:150:ASP:OD1	4:D:151:ASP:N	2.36	0.58
2:B:78:TYR:OH	7:B:302:HOH:O	2.16	0.57
5:E:30:ASN:ND2	7:E:314:HOH:O	2.39	0.54
1:A:212:GLU:CD	7:A:408:HOH:O	2.52	0.52
4:D:178:LYS:NZ	4:D:180:ASP:OD1	2.43	0.51
5:E:185:ASP:N	5:E:185:ASP:OD1	2.45	0.49
4:D:200:SER:HB3	4:D:201:PRO:HD2	1.95	0.49
5:E:129:GLU:CD	7:E:309:HOH:O	2.55	0.49
4:D:15:GLU:OE2	7:D:303:HOH:O	2.20	0.48
2:B:94:LYS:NZ	7:B:303:HOH:O	2.17	0.48
4:D:185:ASN:HB2	7:D:310:HOH:O	2.14	0.48
5:E:227:ARG:NH1	7:E:307:HOH:O	2.33	0.48
4:D:200:SER:O	4:D:201:PRO:C	2.58	0.46
5:E:30:ASN:OD1	7:E:304:HOH:O	2.21	0.46
5:E:207:HIS:NE2	5:E:238:GLU:OE1	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:TRP:HZ2	3:C:9:LEU:HD23	1.83	0.43
5:E:226:ASP:OD1	5:E:227:ARG:N	2.52	0.43
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.55	0.42
5:E:54:VAL:HG13	7:E:384:HOH:O	2.19	0.42
1:A:147:TRP:CZ2	3:C:9:LEU:HD23	2.55	0.41
1:A:121:LYS:HE3	7:A:467:HOH:O	2.20	0.41
1:A:81:LEU:HD13	1:A:118:TYR:CD1	2.55	0.41
1:A:231:VAL:HG11	1:A:244:TRP:CZ2	2.56	0.41
4:D:160:LEU:HD12	4:D:160:LEU:C	2.47	0.40
4:D:148:SER:HB3	7:D:314:HOH:O	2.21	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:574:HOH:O	7:D:384:HOH:O[2_656]	1.84	0.36
7:A:546:HOH:O	7:A:570:HOH:O[2_756]	1.98	0.22
7:B:338:HOH:O	7:D:301:HOH:O[2_756]	2.07	0.13

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	273/275 (99%)	266 (97%)	7 (3%)	0	100	100
2	B	96/98 (98%)	95 (99%)	1 (1%)	0	100	100
3	C	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
4	D	200/200 (100%)	195 (98%)	5 (2%)	0	100	100
5	E	239/241 (99%)	229 (96%)	10 (4%)	0	100	100
All	All	815/823 (99%)	791 (97%)	24 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	231/231 (100%)	230 (100%)	1 (0%)	84	87
2	B	93/93 (100%)	92 (99%)	1 (1%)	65	68
3	C	7/7 (100%)	7 (100%)	0	100	100
4	D	177/177 (100%)	172 (97%)	5 (3%)	38	34
5	E	205/209 (98%)	198 (97%)	7 (3%)	32	27
All	All	713/717 (99%)	699 (98%)	14 (2%)	48	47

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	198	GLU
2	B	94	LYS
4	D	21	PHE
4	D	34	HIS
4	D	83	GLU
4	D	178	LYS
4	D	180	ASP
5	E	3	ILE
5	E	26	GLU
5	E	115	GLU
5	E	177	LEU
5	E	183	LEU
5	E	185	ASP
5	E	193	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN

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Mol	Chain	Res	Type
1	A	197	HIS
2	B	2	GLN
4	D	81	GLN
5	E	19	GLN
5	E	55	ASN
5	E	213	GLN
5	E	233	GLN

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 ⓘ

3 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	$\# Z > 2$
6	GOL	B	101	-	5,5,5	0.35	0	5,5,5	0.48	0
6	GOL	A	301	-	5,5,5	0.41	0	5,5,5	0.40	0
6	GOL	A	302	-	5,5,5	0.44	0	5,5,5	0.72	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
6	GOL	B	101	-	-	3/4/4/4	-
6	GOL	A	301	-	-	1/4/4/4	-
6	GOL	A	302	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	101	GOL	C1-C2-C3-O3
6	B	101	GOL	O2-C2-C3-O3
6	B	101	GOL	O1-C1-C2-O2
6	A	301	GOL	O1-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	302	GOL	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

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	A	275/275 (100%)	-0.19	3 (1%) 78 80	15, 32, 80, 101	0
2	B	98/98 (100%)	-0.29	0 100 100	16, 33, 68, 84	0
3	C	9/9 (100%)	-0.42	0 100 100	19, 22, 28, 35	0
4	D	200/200 (100%)	0.32	12 (6%) 27 27	21, 40, 80, 100	2 (1%)
5	E	241/241 (100%)	0.26	10 (4%) 41 42	22, 49, 87, 106	0
All	All	823/823 (100%)	0.05	25 (3%) 52 53	15, 40, 81, 106	2 (0%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	129	SER	6.8
4	D	131[A]	LYS	4.9
4	D	127	ALA	4.5
4	D	130	ALA	4.0
5	E	180	GLN	3.5
5	E	182	ALA	3.4
4	D	183	CYS	3.4
4	D	201	PRO	3.4
5	E	3	ILE	3.3
5	E	183	LEU	3.3
4	D	126	SER	3.2
4	D	151	ASP	3.1
5	E	243	ALA	3.0
5	E	220	ASN	2.7
1	A	194	VAL	2.6
4	D	83	GLU	2.4
5	E	177	LEU	2.4
5	E	113	VAL	2.3
4	D	128[A]	SER	2.3
4	D	124	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	138	MET	2.1
1	A	136	ALA	2.1
5	E	197	SER	2.1
4	D	165	MET	2.0
5	E	185	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
6	GOL	B	101	6/6	0.81	0.18	19,19,19,19	14
6	GOL	A	301	6/6	0.87	0.12	19,19,19,19	14
6	GOL	A	302	6/6	0.88	0.12	19,19,19,19	14

6.5 Other polymers [i](#)

There are no such residues in this entry.