



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2024 – 07:16 pm BST

PDB ID : 8RYP
Title : Structure of S8 TCR in complex with HLA-A*03:01 bound to ELFSYLIEK peptide
Authors : Karuppiah, V.
Deposited on : 2024-02-09
Resolution : 1.81 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.002 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.38.2

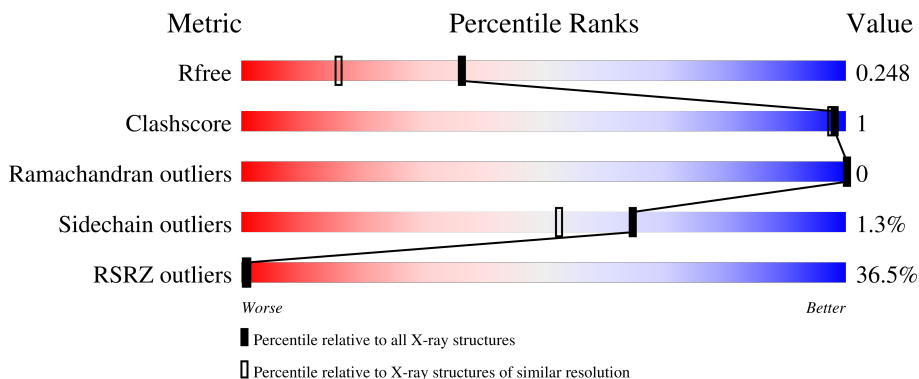
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.81 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}	164625	9242 (1.84-1.80)
Clashscore	180529	1080 (1.82-1.82)
Ramachandran outliers	177936	1073 (1.82-1.82)
Sidechain outliers	177891	1073 (1.82-1.82)
RSRZ outliers	164620	9241 (1.84-1.80)

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	276	 14% 100%
2	B	100	 4% 95%
3	C	9	 78% 22%
4	D	200	 55% 93% 5%
5	E	244	 59% 93%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 6870 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 HLA class I histocompatibility antigen, A alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	276	2252	1401	408	434	9	0	1	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	276	PRO	-	expression tag	UNP P04439

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	100	837	533	141	159	4	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called ELFSYLIEK peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	9	81	55	10	16	0	0	0

- Molecule 4 is a protein called TCR alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	190	1461	903	254	296	8	0	1	0

- Molecule 5 is a protein called TCR beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	237	1881	1189	326	361	5	0	1	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	B	1	4	2	2	0	0

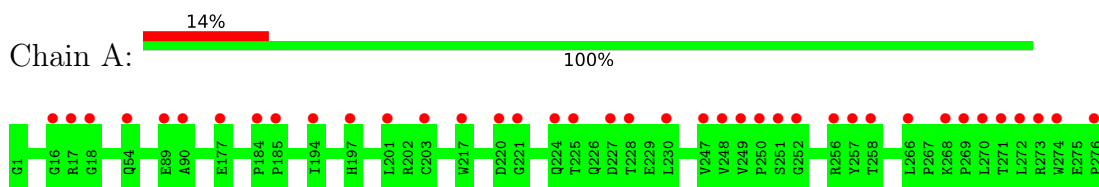
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	159	Total 159	O 159	0	0
7	B	107	Total 107	O 107	0	0
7	C	5	Total 5	O 5	0	0
7	D	39	Total 39	O 39	0	0
7	E	44	Total 44	O 44	0	0

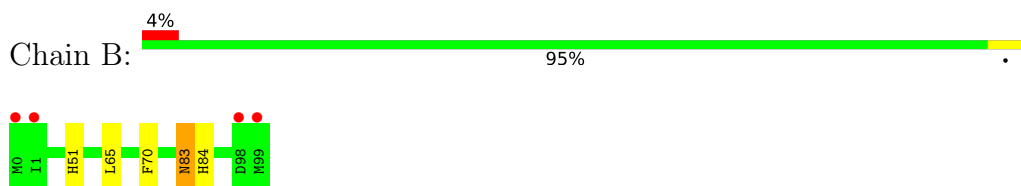
3 Residue-property plots [i](#)

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.

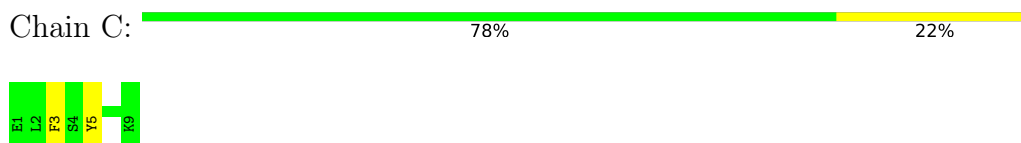
- Molecule 1: HLA class I histocompatibility antigen, A alpha chain



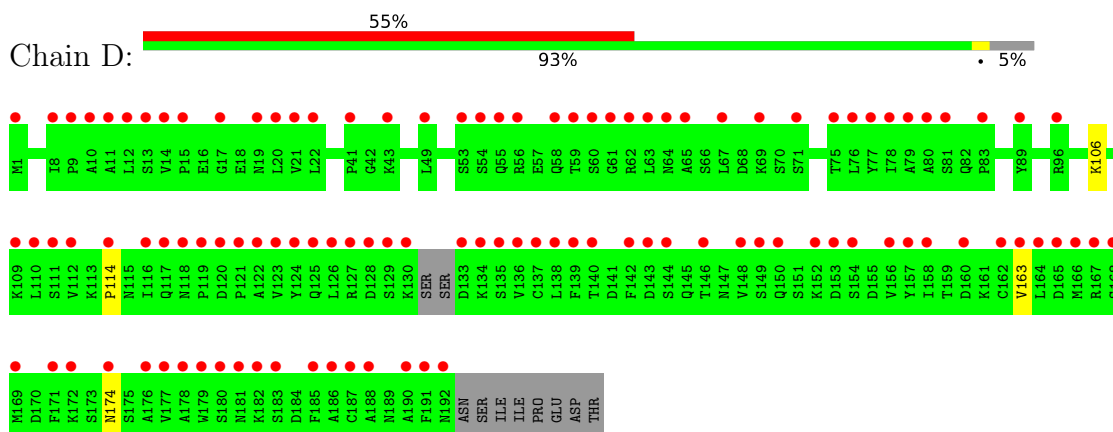
- Molecule 2: Beta-2-microglobulin



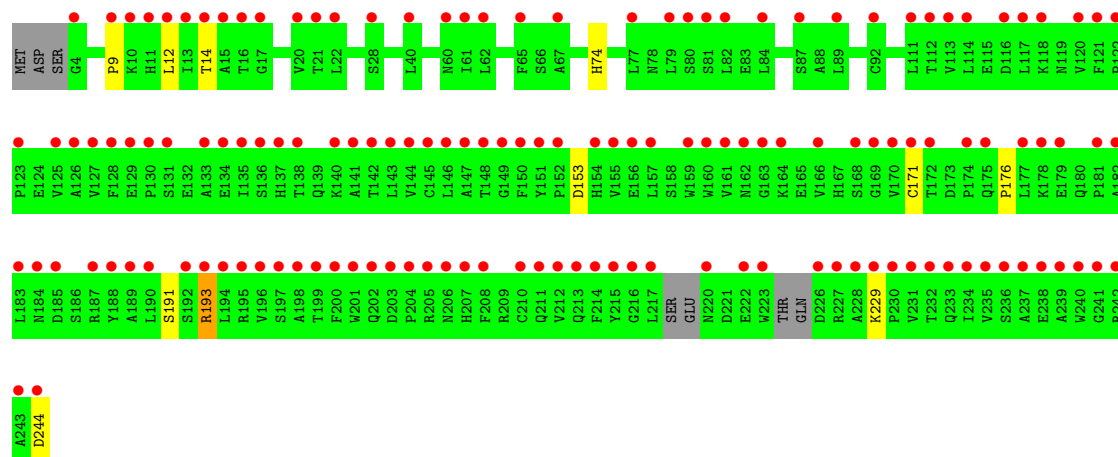
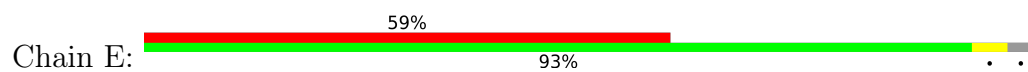
- Molecule 3: ELFSYLIEK peptide



- Molecule 4: TCR alpha



- Molecule 5: TCR beta



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	208.12Å 45.71Å 121.68Å 90.00° 94.93° 90.00°	Depositor
Resolution (Å)	121.23 – 1.81 121.23 – 1.81	Depositor EDS
% Data completeness (in resolution range)	99.9 (121.23-1.81) 99.9 (121.23-1.81)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 1.81Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.221 , 0.241 0.228 , 0.248	Depositor DCC
R_{free} test set	5073 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	34.9	Xtrriage
Anisotropy	0.483	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 37.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6870	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.86% 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: EDO

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	0.62	0/2316	0.71	0/3144
2	B	0.62	0/860	0.71	0/1162
3	C	0.65	0/82	0.69	0/107
4	D	0.66	0/1486	0.73	0/2007
5	E	0.64	0/1934	0.70	0/2631
All	All	0.64	0/6678	0.71	0/9051

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	2252	0	2106	0	0
2	B	837	0	803	2	0
3	C	81	0	83	1	0
4	D	1461	0	1430	2	0
5	E	1881	0	1777	3	0
6	B	4	0	6	0	0
7	A	159	0	0	0	0
7	B	107	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	5	0	0	0	0
7	D	39	0	0	0	0
7	E	44	0	0	0	0
All	All	6870	0	6205	8	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 1.

All (8) 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:C:3:PHE:CZ	3:C:5:TYR:HB3	2.46	0.51
2:B:51:HIS:HA	2:B:65:LEU:O	2.16	0.46
5:E:153:ASP:HB2	5:E:176:PRO:HG2	1.99	0.43
2:B:83:ASN:HD22	2:B:84:HIS:H	1.65	0.43
5:E:9:PRO:HG2	5:E:12:LEU:HG	2.01	0.43
4:D:163:VAL:HG22	4:D:174:ASN:OD1	2.20	0.42
4:D:114:PRO:HG2	4:D:163:VAL:HG11	2.01	0.42
5:E:191:SER:OG	5:E:193:ARG:NH1	2.53	0.42

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	275/276 (100%)	270 (98%)	5 (2%)	0	100	100
2	B	98/100 (98%)	98 (100%)	0	0	100	100
3	C	7/9 (78%)	7 (100%)	0	0	100	100
4	D	187/200 (94%)	183 (98%)	4 (2%)	0	100	100
5	E	232/244 (95%)	225 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	799/829 (96%)	783 (98%)	16 (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	234/233 (100%)	234 (100%)	0	100	100
2	B	95/95 (100%)	93 (98%)	2 (2%)	48	32
3	C	9/9 (100%)	9 (100%)	0	100	100
4	D	167/176 (95%)	166 (99%)	1 (1%)	84	78
5	E	204/211 (97%)	198 (97%)	6 (3%)	37	19
All	All	709/724 (98%)	700 (99%)	9 (1%)	65	52

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	70	PHE
2	B	83	ASN
4	D	106	LYS
5	E	14	THR
5	E	74	HIS
5	E	171	CYS
5	E	193	ARG
5	E	229	LYS
5	E	244	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	HIS
1	A	224	GLN

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Mol	Chain	Res	Type
2	B	83	ASN
5	E	100	HIS
5	E	154	HIS
5	E	202	GLN

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](#)

1 ligand is 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	EDO	B	101	-	3,3,3	0.10	0	2,2,2	0.12	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	B	101	-	-	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.

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	A	276/276 (100%)	0.81	39 (14%) 7 6	20, 43, 88, 101	1 (0%)
2	B	100/100 (100%)	0.38	4 (4%) 43 42	27, 36, 56, 61	0
3	C	9/9 (100%)	-0.05	0 100 100	32, 33, 34, 39	0
4	D	190/200 (95%)	2.26	110 (57%) 0 0	27, 66, 96, 112	1 (0%)
5	E	237/244 (97%)	2.49	143 (60%) 0 0	36, 67, 108, 150	1 (0%)
All	All	812/829 (97%)	1.58	296 (36%) 1 1	20, 53, 96, 150	3 (0%)

All (296) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	240	TRP	6.8
5	E	121	PHE	6.4
5	E	223	TRP	6.2
5	E	117	LEU	6.0
5	E	239	ALA	5.8
5	E	208	PHE	5.5
5	E	237	ALA	5.4
5	E	243	ALA	5.3
5	E	241	GLY	5.2
5	E	212	VAL	5.1
5	E	146	LEU	5.1
5	E	230	PRO	5.0
4	D	138	LEU	5.0
5	E	217	LEU	5.0
4	D	152	LYS	4.9
5	E	183	LEU	4.9
5	E	194	LEU	4.8
5	E	204	PRO	4.8
5	E	144	VAL	4.7
5	E	188	TYR	4.7

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Mol	Chain	Res	Type	RSRZ
5	E	242	ARG	4.7
5	E	128	PHE	4.6
5	E	201	TRP	4.5
5	E	234	ILE	4.5
5	E	216	GLY	4.5
5	E	133	ALA	4.5
5	E	177	LEU	4.5
4	D	124	TYR	4.4
5	E	199	THR	4.4
5	E	120	VAL	4.3
5	E	235	VAL	4.3
5	E	189	ALA	4.3
4	D	171	PHE	4.2
5	E	127	VAL	4.2
5	E	231	VAL	4.2
5	E	150	PHE	4.2
5	E	228	ALA	4.2
1	A	194	ILE	4.2
5	E	236	SER	4.2
5	E	123	PRO	4.2
5	E	154	HIS	4.2
5	E	122	PRO	4.1
4	D	116	ILE	4.1
5	E	181	PRO	4.1
4	D	191	PHE	4.1
5	E	206	ASN	4.0
5	E	14	THR	4.0
4	D	123	VAL	4.0
5	E	126	ALA	4.0
5	E	198	ALA	4.0
5	E	200	PHE	4.0
4	D	164	LEU	4.0
5	E	190	LEU	4.0
4	D	179	TRP	4.0
5	E	141	ALA	4.0
1	A	257	TYR	3.9
5	E	214	PHE	3.9
5	E	15	ALA	3.9
5	E	147	ALA	3.9
5	E	233	GLN	3.9
4	D	158	ILE	3.9
1	A	248	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
5	E	125	VAL	3.8
4	D	182	LYS	3.8
5	E	160	TRP	3.8
2	B	1	ILE	3.8
5	E	84	LEU	3.8
4	D	17	GLY	3.8
5	E	60	ASN	3.8
4	D	21	VAL	3.8
4	D	119	PRO	3.8
5	E	152	PRO	3.8
5	E	163	GLY	3.8
4	D	157	TYR	3.8
5	E	210	CYS	3.7
5	E	215	TYR	3.7
4	D	130	LYS	3.7
4	D	187	CYS	3.7
1	A	270	LEU	3.7
4	D	20	LEU	3.7
5	E	229	LYS	3.7
4	D	61	GLY	3.6
5	E	227	ARG	3.6
5	E	207	HIS	3.6
4	D	67	LEU	3.6
4	D	127	ARG	3.6
1	A	225	THR	3.5
5	E	114	LEU	3.5
4	D	186	ALA	3.5
5	E	155	VAL	3.5
1	A	273	ARG	3.5
4	D	59	THR	3.5
4	D	128	ASP	3.5
4	D	78	ILE	3.4
4	D	168	SER	3.4
4	D	110	LEU	3.4
1	A	16	GLY	3.4
1	A	276	PRO	3.4
4	D	177	VAL	3.4
4	D	188	ALA	3.4
5	E	143	LEU	3.4
5	E	159	TRP	3.3
5	E	196	VAL	3.3
1	A	272	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
5	E	111	LEU	3.3
5	E	161	VAL	3.3
5	E	151	TYR	3.3
5	E	40	LEU	3.3
4	D	134	LYS	3.3
4	D	10	ALA	3.2
5	E	130	PRO	3.2
5	E	92	CYS	3.2
4	D	8	ILE	3.2
5	E	112	THR	3.2
5	E	62	LEU	3.2
1	A	274	TRP	3.2
1	A	18	GLY	3.2
1	A	252	GLY	3.2
5	E	169	GLY	3.2
4	D	111	SER	3.2
5	E	116	ASP	3.2
5	E	166	VAL	3.2
4	D	140	THR	3.2
5	E	164	LYS	3.1
1	A	256	ARG	3.1
5	E	61	ILE	3.1
4	D	14	VAL	3.1
1	A	17	ARG	3.1
5	E	16	THR	3.1
4	D	79	ALA	3.1
4	D	139	PHE	3.1
4	D	76	LEU	3.1
5	E	142	THR	3.1
4	D	142	PHE	3.1
1	A	247	VAL	3.1
4	D	156	VAL	3.1
5	E	13	ILE	3.0
5	E	187	ARG	3.0
5	E	175	GLN	3.0
4	D	63	LEU	3.0
4	D	150	GLN	3.0
5	E	149	GLY	3.0
4	D	112	VAL	3.0
5	E	244	ASP	3.0
4	D	129	SER	3.0
5	E	192	SER	3.0

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Mol	Chain	Res	Type	RSRZ
5	E	197	SER	3.0
5	E	138	THR	3.0
5	E	170	VAL	3.0
5	E	220	ASN	2.9
5	E	203	ASP	2.9
5	E	226	ASP	2.9
4	D	56	ARG	2.9
5	E	136	SER	2.9
5	E	174	PRO	2.9
5	E	145	CYS	2.9
1	A	230	LEU	2.8
4	D	83	PRO	2.8
4	D	166	MET	2.8
4	D	192	ASN	2.8
5	E	17	GLY	2.8
4	D	77	TYR	2.8
1	A	197	HIS	2.8
4	D	181	ASN	2.8
5	E	129	GLU	2.8
4	D	162	CYS	2.8
4	D	58	GLN	2.8
4	D	54	SER	2.8
4	D	80	ALA	2.7
5	E	148	THR	2.7
5	E	162	ASN	2.7
4	D	49	LEU	2.7
4	D	62	ARG	2.7
4	D	160	ASP	2.7
1	A	228	THR	2.7
4	D	19	ASN	2.7
4	D	180	SER	2.7
4	D	153	ASP	2.7
4	D	1	MET	2.7
5	E	238	GLU	2.7
5	E	4	GLY	2.7
1	A	250	PRO	2.7
5	E	184	ASN	2.6
4	D	183	SER	2.6
5	E	82	LEU	2.6
1	A	258	THR	2.6
5	E	113	VAL	2.6
4	D	137	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
5	E	140	LYS	2.6
1	A	201	LEU	2.6
1	A	221	GLY	2.6
5	E	10	LYS	2.6
4	D	121	PRO	2.6
4	D	117	GLN	2.6
4	D	15	PRO	2.5
1	A	251	SER	2.5
4	D	22	LEU	2.5
4	D	154	SER	2.5
4	D	169	MET	2.5
4	D	190	ALA	2.5
1	A	249	VAL	2.5
4	D	55	GLN	2.5
1	A	268	LYS	2.5
4	D	146	THR	2.5
5	E	172	THR	2.5
4	D	178	ALA	2.5
5	E	182	ALA	2.5
5	E	202	GLN	2.5
5	E	222	GLU	2.5
4	D	53	SER	2.5
5	E	193	ARG	2.5
5	E	157	LEU	2.5
4	D	133	ASP	2.4
4	D	143	ASP	2.4
5	E	11	HIS	2.4
5	E	89	LEU	2.4
5	E	131	SER	2.4
1	A	220	ASP	2.4
4	D	144	SER	2.4
4	D	149	SER	2.4
4	D	163	VAL	2.4
5	E	20	VAL	2.4
1	A	271	THR	2.4
2	B	0	MET	2.4
2	B	99	MET	2.4
4	D	81	SER	2.4
4	D	136	VAL	2.4
4	D	176	ALA	2.3
5	E	28	SER	2.3
1	A	224	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
4	D	75	THR	2.3
1	A	266	LEU	2.3
4	D	41	PRO	2.3
4	D	167	ARG	2.3
4	D	148	VAL	2.3
5	E	137	HIS	2.3
1	A	54	GLN	2.3
5	E	22	LEU	2.3
5	E	168	SER	2.3
5	E	179	GLU	2.3
4	D	11	ALA	2.3
4	D	122	ALA	2.3
4	D	109	LYS	2.3
4	D	165	ASP	2.3
5	E	185	ASP	2.3
4	D	89	TYR	2.3
5	E	77	LEU	2.3
5	E	195	ARG	2.2
4	D	9	PRO	2.2
4	D	125	GLN	2.2
5	E	232	THR	2.2
1	A	177	GLU	2.2
4	D	135	SER	2.2
4	D	64	ASN	2.2
1	A	184	PRO	2.2
4	D	114	PRO	2.2
5	E	178	LYS	2.2
1	A	203	CYS	2.2
4	D	71	SER	2.2
5	E	81	SER	2.2
5	E	205	ARG	2.2
5	E	12	LEU	2.2
4	D	172	LYS	2.2
1	A	269	PRO	2.2
5	E	9	PRO	2.2
5	E	135	ILE	2.2
5	E	171	CYS	2.2
5	E	118	LYS	2.2
4	D	174	ASN	2.2
5	E	211	GLN	2.2
1	A	89	GLU	2.2
4	D	43	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
4	D	185	PHE	2.1
5	E	65	PHE	2.1
4	D	60	SER	2.1
1	A	90	ALA	2.1
4	D	12	LEU	2.1
4	D	126	LEU	2.1
1	A	227	ASP	2.1
4	D	120	ASP	2.1
4	D	96	ARG	2.1
4	D	65	ALA	2.1
5	E	67	ALA	2.1
4	D	13	SER	2.1
4	D	69	LYS	2.1
1	A	217	TRP	2.1
5	E	21	THR	2.1
5	E	156	GLU	2.1
2	B	98	ASP	2.0
1	A	185	PRO	2.0
5	E	79	LEU	2.0
5	E	213	GLN	2.0
5	E	134	GLU	2.0
5	E	80[A]	SER	2.0
5	E	87	SER	2.0
4	D	118	ASN	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 monosaccharides 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(\AA^2)	Q<0.9
6	EDO	B	101	4/4	0.83	0.17	38,40,42,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.