



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:28 AM UTC

PDB ID : 4UDU / pdb_00004udu
Title : Crystal structure of staphylococcal enterotoxin E in complex with a T cell receptor
Authors : Rodstrom, K.E.J.; Regenthal, P.; Lindkvist-Petersson, K.
Deposited on : 2014-12-11
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

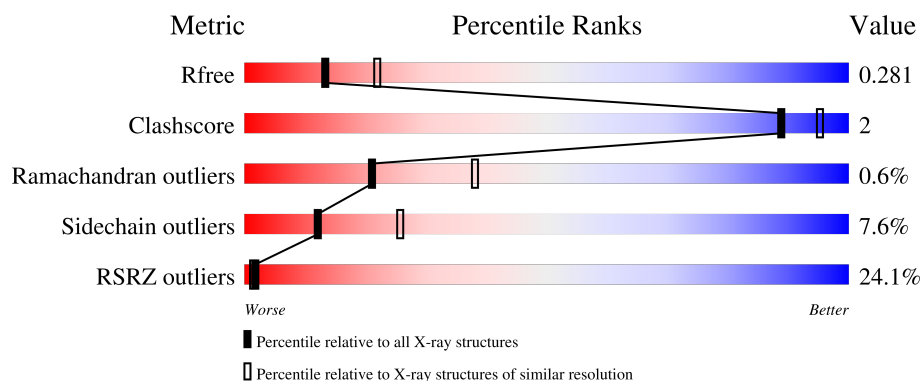
1 Overall quality at a glance

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	A	206	38% 81% 8% 11%
2	B	243	19% 88% 9% ••
3	C	233	13% 83% 9% • 6%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4915 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 T CELL RECEPTOR ALPHA CHAIN, T-CELL RECEPTOR ALPHA CHAIN C REGION.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	184	Total	C	N	O	S	0	0	0
			1315	836	218	254	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	160	CYS	THR	engineered mutation	UNP P01848

- Molecule 2 is a protein called PROTEIN TRBV7-9, T-CELL RECEPTOR BETA-2 CHAIN C REGION.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	238	Total	C	N	O	S	0	0	0
			1848	1166	331	345	6			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP A0A5A3
B	98	GLY	-	linker	UNP A0A5A3
B	99	GLY	-	linker	UNP A0A5A3
B	100	TYR	-	linker	UNP A0A5A3
B	101	GLU	-	linker	UNP A0A5A3
B	102	GLN	-	linker	UNP A0A5A3
B	103	TYR	-	linker	UNP A0A5A3
B	104	PHE	-	linker	UNP A0A5A3
B	105	GLY	-	linker	UNP A0A5A3
B	106	PRO	-	linker	UNP A0A5A3
B	107	GLY	-	linker	UNP A0A5A3
B	108	THR	-	linker	UNP A0A5A3
B	109	ARG	-	linker	UNP A0A5A3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	110	LEU	-	linker	UNP A0A5A3
B	111	THR	-	linker	UNP A0A5A3
B	112	VAL	-	linker	UNP A0A5A3
B	113	THR	-	linker	UNP A0A5A3
B	114	GLU	-	linker	UNP A0A5A3
B	128	VAL	GLU	engineered mutation	UNP A0A5B9
B	170	CYS	SER	engineered mutation	UNP A0A5B9
B	188	ALA	CYS	engineered mutation	UNP A0A5B9
B	202	ASP	ASN	engineered mutation	UNP A0A5B9

- Molecule 3 is a protein called ENTEROTOXIN TYPE E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	218	Total	C	N	O	S	0	0	0
			1699	1084	292	320	3			

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Zn	0	0
			1	1		

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	2	Total	Na	0	0
			2	2		

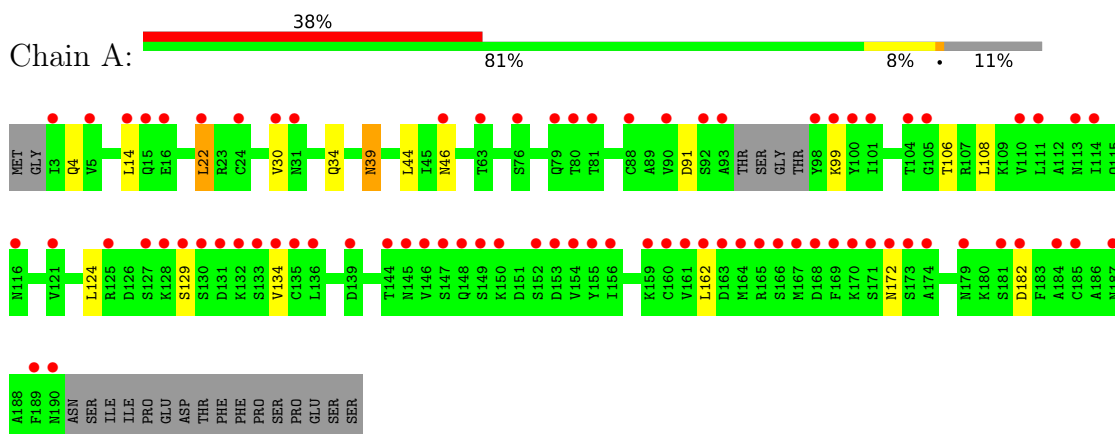
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	9	Total	O	0	0
			9	9		
6	B	15	Total	O	0	0
			15	15		
6	C	26	Total	O	0	0
			26	26		

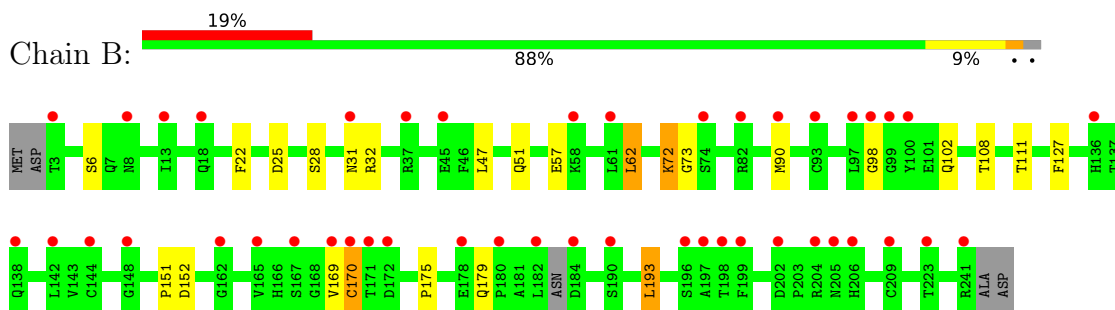
3 Residue-property plots [i](#)

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.

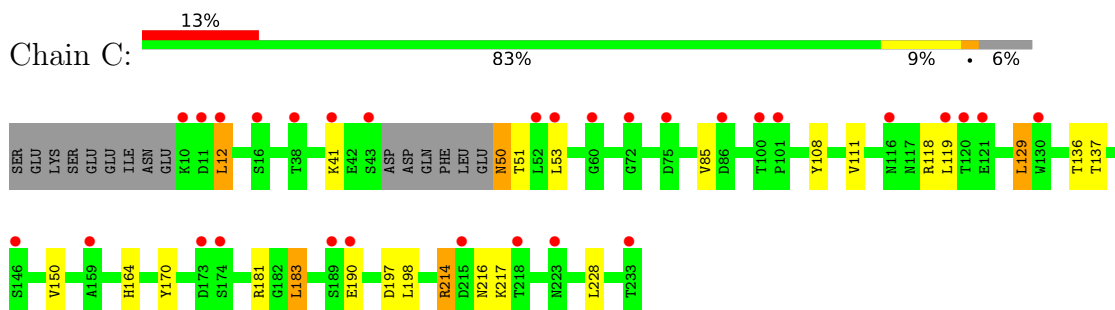
- Molecule 1: T CELL RECEPTOR ALPHA CHAIN, T-CELL RECEPTOR ALPHA CHAIN C REGION



- Molecule 2: PROTEIN TRBV7-9, T-CELL RECEPTOR BETA-2 CHAIN C REGION



- Molecule 3: ENTEROTOXIN TYPE E



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.13Å 78.54Å 180.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.33 – 2.50 32.33 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.4 (32.33-2.50) 97.4 (32.33-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.51Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.246 , 0.255 0.261 , 0.281	Depositor DCC
R_{free} test set	1597 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	52.9	Xtriage
Anisotropy	0.563	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4915	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% 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: ZN, NA

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	0.69	0/1341	1.09	1/1835 (0.1%)
2	B	0.63	0/1899	1.08	0/2587
3	C	0.64	0/1735	1.19	1/2349 (0.0%)
All	All	0.65	0/4975	1.12	2/6771 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	197	ASP	CA-CB-CG	5.46	118.06	112.60
1	A	39	ASN	CA-CB-CG	5.17	117.77	112.60

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	1315	0	1156	4	0
2	B	1848	0	1702	11	0
3	C	1699	0	1608	6	0
4	C	1	0	0	0	0
5	C	2	0	0	0	0
6	A	9	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	15	0	0	0	0
6	C	26	0	0	0	0
All	All	4915	0	4466	18	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 2.

All (18) 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:164:HIS:HD2	3:C:170:TYR:H	1.34	0.75
3:C:111:VAL:H	3:C:216:ASN:HD21	1.51	0.59
2:B:47:LEU:HB3	2:B:62:LEU:HD23	1.92	0.51
1:A:162:LEU:HD12	2:B:170:CYS:HB2	1.92	0.51
1:A:22:LEU:HD12	1:A:106:THR:HG21	1.93	0.51
2:B:152:ASP:HB2	2:B:175:PRO:HG2	1.95	0.48
2:B:22:PHE:CD1	2:B:108:THR:HG21	2.49	0.47
3:C:50:ASN:HD22	3:C:51:THR:HG23	1.79	0.47
2:B:169:VAL:HG22	2:B:193:LEU:HD23	1.98	0.46
2:B:111:THR:HG21	2:B:151:PRO:HB3	1.98	0.45
1:A:34:GLN:HE22	2:B:102:GLN:HB2	1.83	0.43
2:B:32:ARG:HG2	2:B:51:GLN:HG3	1.99	0.42
2:B:6:SER:HB2	2:B:25:ASP:HB2	2.01	0.42
3:C:12:LEU:HD11	3:C:183:LEU:HG	2.02	0.42
1:A:124:LEU:HB3	2:B:127:PHE:HB3	2.01	0.41
3:C:108:TYR:CD1	3:C:214:ARG:HG2	2.55	0.41
3:C:129:LEU:HD23	3:C:228:LEU:HB3	2.02	0.40
2:B:72:LYS:HA	2:B:73:GLY:HA2	1.61	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	180/206 (87%)	171 (95%)	7 (4%)	2 (1%)	11	22
2	B	234/243 (96%)	222 (95%)	10 (4%)	2 (1%)	14	27
3	C	214/233 (92%)	204 (95%)	10 (5%)	0	100	100
All	All	628/682 (92%)	597 (95%)	27 (4%)	4 (1%)	21	38

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	129	SER
1	A	182	ASP
2	B	72	LYS
2	B	98	GLY

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	125/185 (68%)	113 (90%)	12 (10%)	8	17
2	B	189/213 (89%)	181 (96%)	8 (4%)	26	52
3	C	172/207 (83%)	155 (90%)	17 (10%)	7	16
All	All	486/605 (80%)	449 (92%)	37 (8%)	12	26

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	14	LEU
1	A	22	LEU
1	A	30	VAL
1	A	39	ASN
1	A	44	LEU
1	A	46	ASN
1	A	91	ASP
1	A	99	LYS

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Mol	Chain	Res	Type
1	A	108	LEU
1	A	134	VAL
1	A	172	ASN
2	B	28	SER
2	B	31	ASN
2	B	57	GLU
2	B	62	LEU
2	B	90	MET
2	B	170	CYS
2	B	179	GLN
2	B	193	LEU
3	C	12	LEU
3	C	41	LYS
3	C	50	ASN
3	C	53	LEU
3	C	85	VAL
3	C	118	ARG
3	C	119	LEU
3	C	129	LEU
3	C	136	THR
3	C	137	THR
3	C	150	VAL
3	C	181	ARG
3	C	183	LEU
3	C	190	GLU
3	C	198	LEU
3	C	214	ARG
3	C	217	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	34	GLN
2	B	31	ASN
2	B	55	GLN
2	B	81	GLN
2	B	118	ASN
2	B	212	GLN
3	C	40	ASN
3	C	50	ASN
3	C	65	ASN

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Mol	Chain	Res	Type
3	C	78	ASN
3	C	158	GLN
3	C	164	HIS
3	C	202	GLN
3	C	204	GLN
3	C	216	ASN

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 3 ligands modelled in this entry, 3 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	184/206 (89%)	2.14	79 (42%) 0 0	24, 75, 105, 125	6 (3%)
2	B	238/243 (97%)	1.45	45 (18%) 3 2	22, 61, 86, 118	10 (4%)
3	C	218/233 (93%)	0.96	30 (13%) 6 5	36, 60, 87, 111	0
All	All	640/682 (93%)	1.48	154 (24%) 2 1	22, 63, 98, 125	16 (2%)

All (154) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	113	ASN	11.6
1	A	63	THR	11.2
1	A	31	ASN	10.8
1	A	15	GLN	10.3
1	A	24	CYS	10.1
2	B	144	CYS	9.7
2	B	31	ASN	9.3
2	B	170	CYS	8.5
2	B	93	CYS	8.4
2	B	209	CYS	8.0
2	B	8	ASN	7.6
2	B	18	GLN	7.5
1	A	98	TYR	6.8
2	B	190	SER	6.6
1	A	88	CYS	6.3
1	A	93	ALA	6.3
1	A	129	SER	5.3
2	B	182	LEU	5.3
3	C	43	SER	5.0
1	A	146	VAL	4.5
1	A	3	ILE	4.4
2	B	74	SER	4.4
2	B	98	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	100	TYR	4.3
1	A	165	ARG	4.3
1	A	150	LYS	4.2
1	A	5	VAL	4.2
1	A	160	CYS	4.1
1	A	90	VAL	4.1
2	B	184	ASP	4.0
2	B	204	ARG	3.9
2	B	198	THR	3.9
2	B	100	TYR	3.9
1	A	99	LYS	3.8
2	B	3	THR	3.7
1	A	92	SER	3.6
1	A	169	PHE	3.6
3	C	53	LEU	3.6
3	C	101	PRO	3.6
1	A	173	SER	3.5
2	B	202	ASP	3.5
1	A	185	CYS	3.5
1	A	147	SER	3.5
1	A	149	SER	3.4
1	A	130	SER	3.4
2	B	241	ARG	3.4
1	A	170	LYS	3.3
3	C	16	SER	3.3
1	A	190	ASN	3.3
2	B	99	GLY	3.3
1	A	181	SER	3.3
1	A	153	ASP	3.2
2	B	37	ARG	3.2
1	A	81	THR	3.1
2	B	61	LEU	3.1
1	A	172	ASN	3.1
1	A	182	ASP	3.1
3	C	119	LEU	3.1
1	A	187	ASN	3.1
1	A	155	TYR	3.0
1	A	162	LEU	3.0
1	A	135	CYS	3.0
1	A	168	ASP	3.0
3	C	11	ASP	3.0
3	C	218	THR	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	197	ALA	2.9
1	A	163	ASP	2.9
3	C	116	ASN	2.9
3	C	120	THR	2.9
1	A	184	ALA	2.9
1	A	148	GLN	2.9
3	C	52	LEU	2.9
2	B	90	MET	2.8
1	A	14	LEU	2.8
1	A	134	VAL	2.8
1	A	161	VAL	2.8
2	B	142	LEU	2.8
1	A	116	ASN	2.8
2	B	205	ASN	2.7
2	B	165	VAL	2.7
2	B	82	ARG	2.7
2	B	136	HIS	2.7
3	C	223	ASN	2.7
1	A	166	SER	2.7
1	A	80	THR	2.7
1	A	145	ASN	2.6
2	B	171	THR	2.6
2	B	178	GLU	2.6
1	A	154	VAL	2.6
1	A	133	SER	2.6
3	C	189	SER	2.5
2	B	58	LYS	2.5
3	C	215	ASP	2.5
1	A	101	ILE	2.5
3	C	130	TRP	2.5
1	A	104	THR	2.5
3	C	146	SER	2.5
3	C	233	THR	2.5
3	C	190	GLU	2.5
1	A	179	ASN	2.5
2	B	169	VAL	2.5
1	A	111	LEU	2.4
1	A	46	ASN	2.4
1	A	110	VAL	2.4
2	B	13	ILE	2.4
1	A	164	MET	2.4
1	A	76	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	136	LEU	2.4
2	B	199	PHE	2.4
1	A	128	LYS	2.4
3	C	121	GLU	2.4
1	A	127	SER	2.4
1	A	156	ILE	2.4
1	A	30	VAL	2.4
1	A	144	THR	2.3
3	C	60	GLY	2.3
2	B	223	THR	2.3
1	A	114	ILE	2.3
3	C	12	LEU	2.3
1	A	131	ASP	2.3
3	C	159	ALA	2.3
2	B	206	HIS	2.3
1	A	22	LEU	2.2
2	B	172	ASP	2.2
3	C	38	THR	2.2
3	C	100	THR	2.2
1	A	167	MET	2.2
2	B	196	SER	2.2
3	C	173	ASP	2.2
2	B	180	PRO	2.2
3	C	72	GLY	2.2
1	A	16	GLU	2.2
1	A	189	PHE	2.2
1	A	174	ALA	2.2
3	C	41	LYS	2.2
3	C	174	SER	2.2
1	A	132	LYS	2.2
1	A	159	LYS	2.2
2	B	138	GLN	2.1
1	A	171	SER	2.1
3	C	75	ASP	2.1
1	A	125	ARG	2.1
2	B	167	SER	2.1
3	C	86	ASP	2.1
1	A	121	VAL	2.1
1	A	79	GLN	2.1
1	A	105	GLY	2.0
2	B	45	GLU	2.0
2	B	148	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	139	ASP	2.0
2	B	97	LEU	2.0
2	B	162	GLY	2.0
3	C	10	LYS	2.0
1	A	152	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($\text{\AA}^2$)	Q<0.9
5	NA	C	1236	1/1	0.91	0.20	59,59,59,59	0
5	NA	C	1235	1/1	0.93	0.17	47,47,47,47	0
4	ZN	C	1234	1/1	0.94	0.08	69,69,69,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.