



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 09:21 am BST

PDB ID : 5NHT
Title : human 199.54-16 TCR in complex with Melan-A/MART-1 (26-35) peptide and HLA-A2
Authors : Exertier, C.; Reiser, J.-B.; Lantez, V.; Chouquet, A.; Bonneville, M.; Saulquin, X.; Housset, D.
Deposited on : 2017-03-22
Resolution : 3.20 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

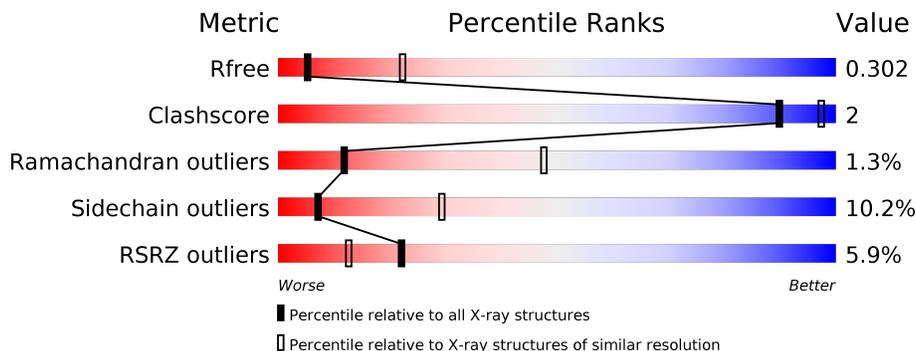
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 on 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	H	276	 3% 88% 12%
2	L	100	 % 85% 14% •
3	P	10	 90% 10%
4	A	211	 11% 78% 14% • 7%
5	B	251	 7% 81% 15% ••

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 6613 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-2 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	H	275	2248	1405	409	425	9	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	245	VAL	ALA	conflict	UNP P01892

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	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
L	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called Melanoma antigen recognized by T-cells 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	P	10	69	45	10	14	0	0	0

- Molecule 4 is a protein called T-cell receptor alpha variable 12-2, T-cell receptor, sp3.4 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	A	197	1521	948	251	314	8	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP A0A075B6T6
A	49	SER	PHE	conflict	UNP A0A075B6T6
A	92	GLY	ASN	linker	UNP A0A075B6T6
A	203	ASN	-	expression tag	UNP K7N5N2
A	204	ASP	-	expression tag	UNP K7N5N2
A	205	GLY	-	expression tag	UNP K7N5N2
A	206	GLY	-	expression tag	UNP K7N5N2
A	207	GLY	-	expression tag	UNP K7N5N2
A	208	CYS	-	expression tag	UNP K7N5N2
A	209	LYS	-	expression tag	UNP K7N5N2

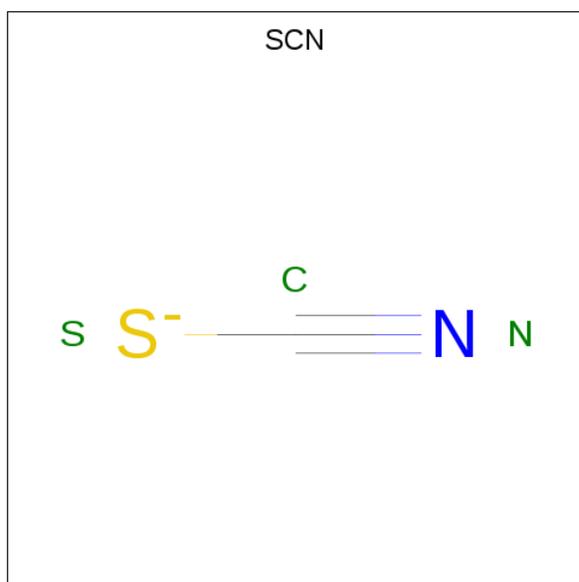
- Molecule 5 is a protein called T-cell receptor beta variable 19,TRB protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	B	243	1931	1219	334	371	7	0	0	1

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	2	MET	-	initiating methionine	UNP A0A5B3
B	95	GLN	-	linker	UNP A0A5B3
B	96	GLY	-	linker	UNP A0A5B3
B	97	LEU	-	linker	UNP A0A5B3
B	98	ALA	-	linker	UNP A0A5B3
B	99	GLY	-	linker	UNP A0A5B3
B	100	ALA	-	linker	UNP A0A5B3
B	171	CYS	SER	conflict	UNP A0A0C4ZKA8
B	245	GLN	-	expression tag	UNP A0A0C4ZKA8
B	246	ASP	-	expression tag	UNP A0A0C4ZKA8
B	247	ARG	-	expression tag	UNP A0A0C4ZKA8
B	248	GLY	-	expression tag	UNP A0A0C4ZKA8
B	249	GLY	-	expression tag	UNP A0A0C4ZKA8
B	250	GLY	-	expression tag	UNP A0A0C4ZKA8
B	251	CYS	-	expression tag	UNP A0A0C4ZKA8
B	252	ASP	-	expression tag	UNP A0A0C4ZKA8

- Molecule 6 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
6	H	1	Total	C	N	S	0	0
			3	1	1	1		

- Molecule 7 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	H	2	Total	K	0	0
			2	2		

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	H	1	Total	Cl	0	0
			1	1		

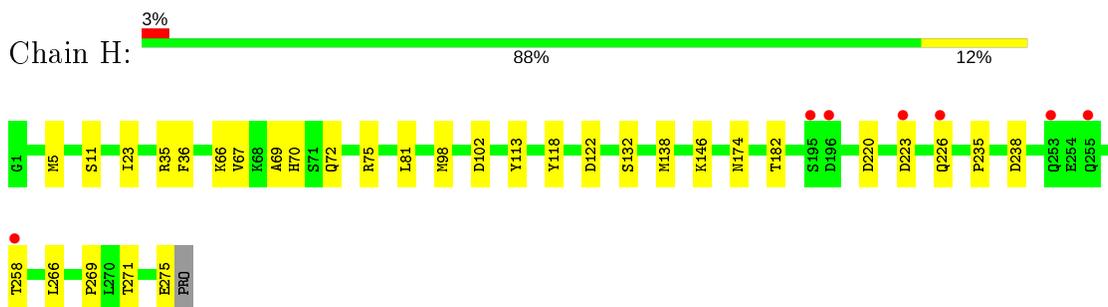
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	H	1	Total	O	0	0
			1	1		

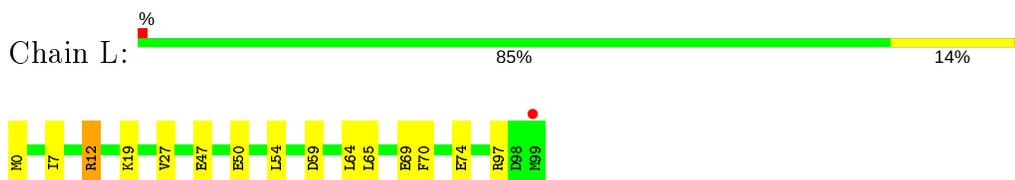
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

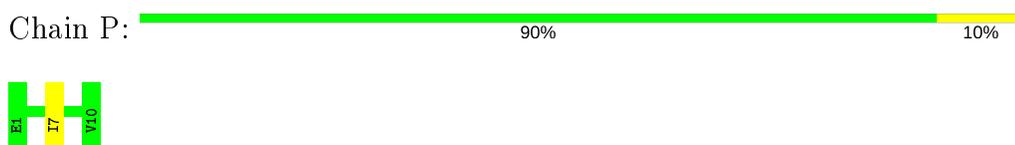
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



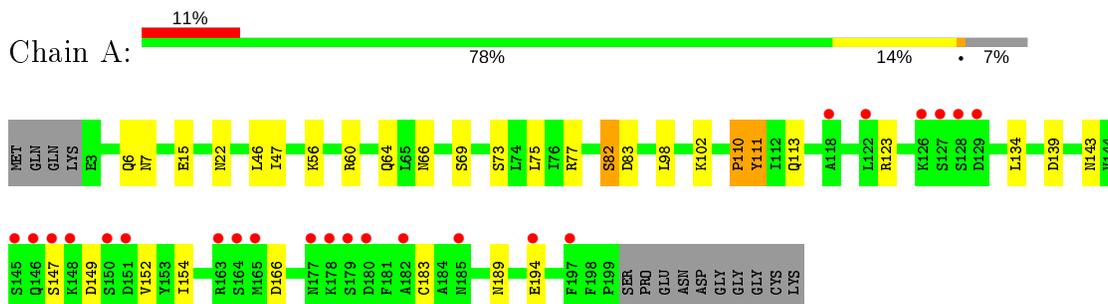
- Molecule 2: Beta-2-microglobulin



- Molecule 3: Melanoma antigen recognized by T-cells 1

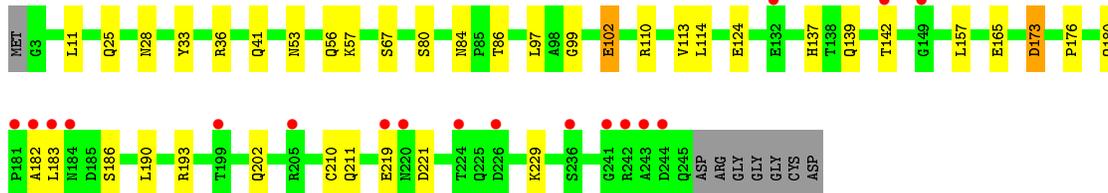


- Molecule 4: T-cell receptor alpha variable 12-2, T-cell receptor, sp3.4 alpha chain



- Molecule 5: T-cell receptor beta variable 19, TRB protein

Chain B:  7% 81% 15%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	222.08 Å 49.28 Å 96.13 Å 90.00° 97.61° 90.00°	Depositor
Resolution (Å)	16.00 – 3.20 15.82 – 3.20	Depositor EDS
% Data completeness (in resolution range)	90.2 (16.00-3.20) 91.1 (15.82-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 3.19 Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.213 , 0.299 0.216 , 0.302	Depositor DCC
R_{free} test set	871 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	53.1	Xtrriage
Anisotropy	0.987	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 64.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6613	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.12% 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: K, SCN, CL

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	H	0.44	0/2313	0.68	0/3140
2	L	0.44	0/860	0.71	1/1162 (0.1%)
3	P	0.43	0/68	0.85	0/90
4	A	0.49	0/1554	0.68	0/2106
5	B	0.48	0/1982	0.70	0/2694
All	All	0.47	0/6777	0.69	1/9192 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	12	ARG	NE-CZ-NH1	5.04	122.82	120.30

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	H	2248	0	2100	6	0
2	L	837	0	803	4	0
3	P	69	0	79	1	0
4	A	1521	0	1427	7	0
5	B	1931	0	1833	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	H	3	0	0	0	0
7	H	2	0	0	0	0
8	H	1	0	0	0	0
9	H	1	0	0	0	0
All	All	6613	0	6242	23	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 (23) 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:P:7:ILE:HB	5:B:97:LEU:HD11	1.79	0.65
4:A:46:LEU:HD22	5:B:102:GLU:HG2	1.82	0.61
5:B:157:LEU:HD12	5:B:190:LEU:HD23	1.88	0.55
4:A:60:ARG:NH2	4:A:83:ASP:OD2	2.41	0.54
5:B:56:GLN:HE21	5:B:57:LYS:N	2.05	0.53
5:B:86:THR:OG1	5:B:113:VAL:HG23	2.10	0.52
1:H:66:LYS:O	1:H:70:HIS:ND1	2.40	0.51
5:B:56:GLN:HE21	5:B:57:LYS:H	1.57	0.50
4:A:15:GLU:HG3	4:A:110:PRO:HA	1.93	0.48
4:A:98:LEU:HD13	5:B:99:GLY:HA2	1.95	0.48
4:A:134:LEU:HD11	5:B:142:THR:HG21	1.98	0.46
1:H:69:ALA:HA	1:H:72:GLN:HE21	1.81	0.46
1:H:258:THR:HB	1:H:271:THR:HG23	2.00	0.43
2:L:7:ILE:HG12	2:L:27:VAL:HG12	2.00	0.43
1:H:81:LEU:HD13	1:H:118:TYR:CD1	2.53	0.43
4:A:149:ASP:HB2	4:A:152:VAL:HG23	2.01	0.42
5:B:221:ASP:O	5:B:229:LYS:NZ	2.51	0.42
1:H:235:PRO:HG2	2:L:65:LEU:HD22	2.02	0.42
1:H:23:ILE:HA	1:H:36:PHE:O	2.20	0.41
2:L:54:LEU:HA	2:L:64:LEU:CD2	2.51	0.41
4:A:147:SER:HA	4:A:154:ILE:HD12	2.02	0.41
5:B:41:GLN:OE1	5:B:41:GLN:N	2.53	0.41
2:L:54:LEU:HA	2:L:64:LEU:HD21	2.03	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	H	273/276 (99%)	240 (88%)	30 (11%)	3 (1%)	14	51
2	L	98/100 (98%)	93 (95%)	4 (4%)	1 (1%)	15	54
3	P	8/10 (80%)	7 (88%)	1 (12%)	0	100	100
4	A	195/211 (92%)	169 (87%)	23 (12%)	3 (2%)	10	44
5	B	241/251 (96%)	199 (83%)	38 (16%)	4 (2%)	9	42
All	All	815/848 (96%)	708 (87%)	96 (12%)	11 (1%)	12	47

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	269	PRO
4	A	82	SER
4	A	110	PRO
4	A	111	TYR
5	B	80	SER
1	H	223	ASP
1	H	238	ASP
5	B	176	PRO
5	B	182	ALA
2	L	59	ASP
5	B	173	ASP

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	H	232/233 (100%)	214 (92%)	18 (8%)	12	43
2	L	95/95 (100%)	86 (90%)	9 (10%)	8	32
3	P	7/7 (100%)	7 (100%)	0	100	100
4	A	172/183 (94%)	150 (87%)	22 (13%)	4	20
5	B	209/215 (97%)	185 (88%)	24 (12%)	5	24
All	All	715/733 (98%)	642 (90%)	73 (10%)	7	29

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	5	MET
1	H	11	SER
1	H	35	ARG
1	H	67	VAL
1	H	75	ARG
1	H	98	MET
1	H	102	ASP
1	H	113	TYR
1	H	122	ASP
1	H	132	SER
1	H	138	MET
1	H	146	LYS
1	H	174	ASN
1	H	182	THR
1	H	220	ASP
1	H	226	GLN
1	H	266	LEU
1	H	275	GLU
2	L	0	MET
2	L	12	ARG
2	L	19	LYS
2	L	47	GLU
2	L	50	GLU
2	L	69	GLU
2	L	70	PHE
2	L	74	GLU
2	L	97	ARG
4	A	6	GLN
4	A	7	ASN
4	A	22	ASN
4	A	47	ILE

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Mol	Chain	Res	Type
4	A	56	LYS
4	A	64	GLN
4	A	66	ASN
4	A	69	SER
4	A	73	SER
4	A	75	LEU
4	A	77	ARG
4	A	82	SER
4	A	102	LYS
4	A	111	TYR
4	A	113	GLN
4	A	123	ARG
4	A	139	ASP
4	A	143	ASN
4	A	166	ASP
4	A	183	CYS
4	A	189	ASN
4	A	194	GLU
5	B	11	LEU
5	B	25	GLN
5	B	28	ASN
5	B	33	TYR
5	B	36	ARG
5	B	53	ASN
5	B	67	SER
5	B	84	ASN
5	B	102	GLU
5	B	110	ARG
5	B	114	LEU
5	B	124	GLU
5	B	137	HIS
5	B	139	GLN
5	B	165	GLU
5	B	173	ASP
5	B	180	GLN
5	B	183	LEU
5	B	186	SER
5	B	193	ARG
5	B	202	GLN
5	B	210	CYS
5	B	211	GLN
5	B	219	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	72	GLN
1	H	174	ASN
1	H	180	GLN
2	L	17	ASN
4	A	66	ASN
4	A	141	GLN
5	B	25	GLN
5	B	56	GLN
5	B	162	ASN
5	B	211	GLN
5	B	213	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

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	SCN	H	301	-	1,2,2	0.33	0	0,1,1	0.00	-

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	H	275/276 (99%)	-0.14	7 (2%) 57 43	29, 61, 125, 148	0
2	L	100/100 (100%)	-0.53	1 (1%) 82 72	31, 45, 86, 103	0
3	P	10/10 (100%)	-0.59	0 100 100	47, 52, 54, 57	0
4	A	197/211 (93%)	0.39	23 (11%) 4 2	34, 68, 153, 181	0
5	B	243/251 (96%)	0.24	18 (7%) 14 8	34, 86, 133, 168	0
All	All	825/848 (97%)	0.04	49 (5%) 22 13	29, 62, 139, 181	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	128	SER	6.3
4	A	150	SER	5.7
4	A	177	ASN	5.7
4	A	129	ASP	4.8
4	A	164	SER	4.8
5	B	199	THR	4.5
4	A	127	SER	4.5
4	A	146	GLN	4.2
4	A	178	LYS	4.2
5	B	224	THR	3.8
4	A	180	ASP	3.7
5	B	183	LEU	3.7
5	B	244	ASP	3.6
4	A	147	SER	3.6
4	A	163	ARG	3.5
5	B	142	THR	3.5
5	B	243	ALA	3.5
1	H	195	SER	3.3
5	B	220	ASN	3.3
4	A	151	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
4	A	185	ASN	3.1
4	A	197	PHE	3.0
5	B	181	PRO	3.0
4	A	118	ALA	3.0
5	B	205	ARG	3.0
5	B	182	ALA	2.9
1	H	253	GLN	2.9
1	H	196	ASP	2.9
4	A	165	MET	2.8
4	A	126	LYS	2.8
4	A	194	GLU	2.8
5	B	241	GLY	2.8
4	A	145	SER	2.6
5	B	242	ARG	2.6
5	B	149	GLY	2.5
4	A	148	LYS	2.5
5	B	132	GLU	2.4
5	B	236	SER	2.3
5	B	184	ASN	2.3
1	H	258	THR	2.3
4	A	179	SER	2.2
1	H	226	GLN	2.2
1	H	255	GLN	2.2
1	H	223	ASP	2.1
5	B	219	GLU	2.1
5	B	226	ASP	2.1
4	A	182	ALA	2.1
2	L	99	MET	2.1
4	A	122	LEU	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 carbohydrates 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(Å ²)	Q<0.9
8	CL	H	304	1/1	0.85	0.27	69,69,69,69	0
7	K	H	303	1/1	0.88	0.24	69,69,69,69	0
6	SCN	H	301	3/3	0.92	0.17	49,49,51,51	0
7	K	H	302	1/1	0.94	0.06	66,66,66,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.