



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:04 PM UTC

PDB ID : 3PWP / pdb_00003pwp
Title : The complex between TCR A6 and human Class I MHC HLA-A2 with the bound HuD peptide
Authors : Borbulevych, O.Y.; Baker, B.M.
Deposited on : 2010-12-08
Resolution : 2.69 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

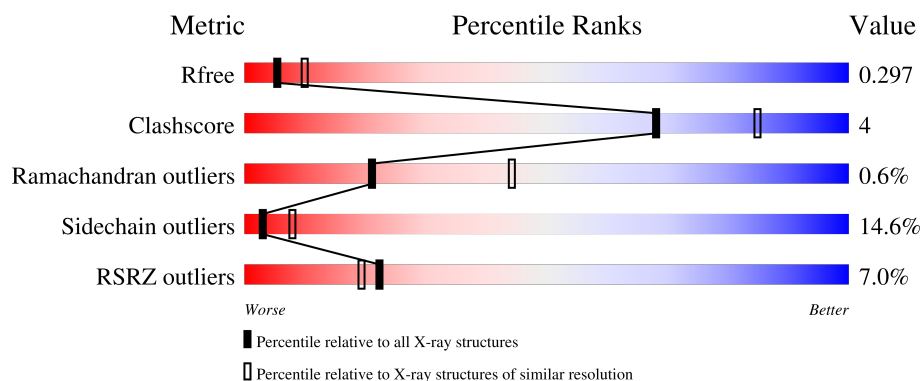
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	12% 82% 15% .
2	B	100	4% 80% 13% 7%
3	C	9	67% 22% 11%
4	D	200	6% 78% 18% ..
5	E	245	3% 77% 20% .

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6757 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
1	A	275	Total	C	N	O	S	0	0	0
			2247	1403	409	426	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	1	0
			843	537	142	160	4			

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 HuD peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			75	52	10	13			

- Molecule 4 is a protein called A6 TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	200	Total	C	N	O	S	0	0	0
			1552	965	255	325	7			

- Molecule 5 is a protein called A6 TCR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	245	Total	C	N	O	S	0	0	0
			1927	1209	338	372	8			

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	E	1	Total	C	O	0	0
			6	3	3		
6	E	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	O	S	0	0
			5	4	1		

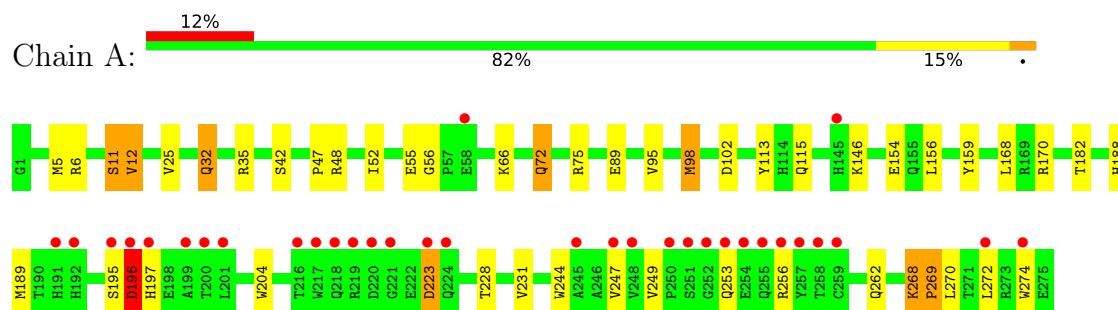
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	19	Total	O	0	0
			19	19		
8	B	16	Total	O	0	0
			16	16		
8	D	7	Total	O	0	0
			7	7		
8	E	24	Total	O	0	0
			24	24		

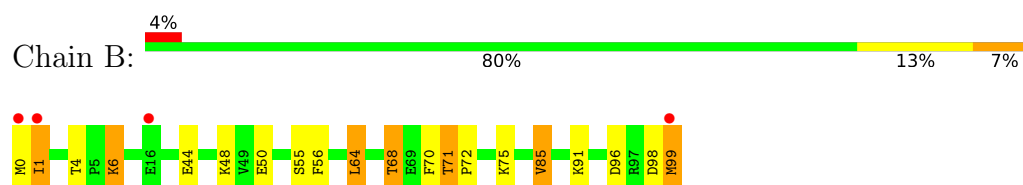
3 Residue-property plots [i](#)

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.

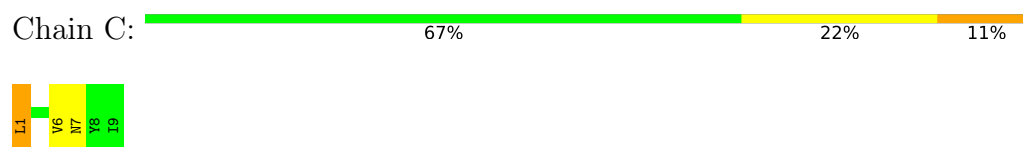
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



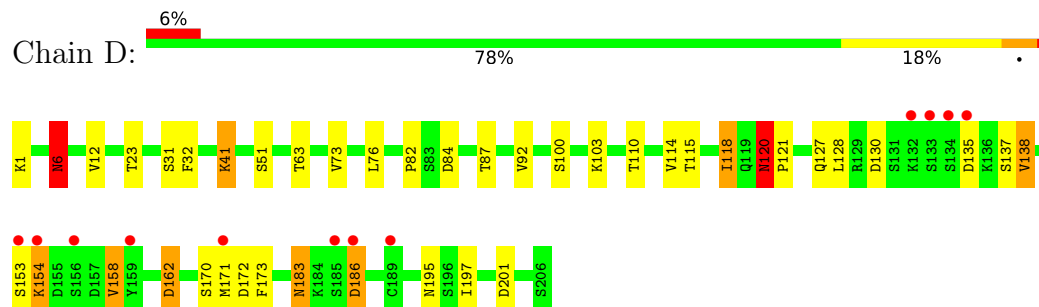
- Molecule 2: Beta-2-microglobulin



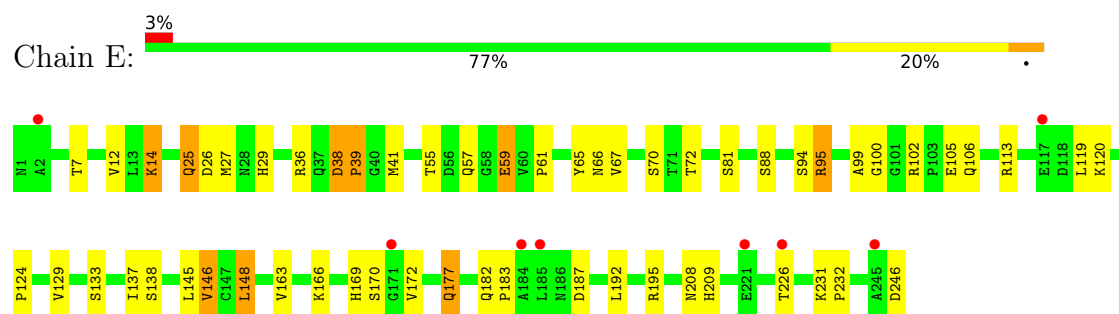
- Molecule 3: HuD peptide



- Molecule 4: A6 TCR alpha chain



- Molecule 5: A6 TCR beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	224.01Å 49.06Å 93.71Å 90.00° 90.07° 90.00°	Depositor
Resolution (Å)	20.00 – 2.69 20.00 – 2.69	Depositor EDS
% Data completeness (in resolution range)	94.2 (20.00-2.69) 93.9 (20.00-2.69)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.88 (at 2.71Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.198 , 0.259 0.254 , 0.297	Depositor DCC
R_{free} test set	1371 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	58.5	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 23.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6757	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 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	0.82	1/2312 (0.0%)	1.14	10/3137 (0.3%)
2	B	0.79	0/869	1.13	4/1174 (0.3%)
3	C	0.93	0/77	0.88	0/102
4	D	0.78	0/1585	1.18	8/2150 (0.4%)
5	E	0.79	1/1980 (0.1%)	1.18	8/2699 (0.3%)
All	All	0.80	2/6823 (0.0%)	1.16	30/9262 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
5	E	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	95	ARG	N-CA	5.57	1.51	1.45
1	A	12	VAL	CA-CB	5.54	1.61	1.54

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	GLY	CA-C-N	9.54	129.16	119.24
1	A	56	GLY	C-N-CA	9.54	129.16	119.24
4	D	120	ASN	CA-C-N	9.20	129.27	119.89
4	D	120	ASN	C-N-CA	9.20	129.27	119.89
5	E	38	ASP	CA-C-N	8.88	130.94	119.84
5	E	38	ASP	C-N-CA	8.88	130.94	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	169	HIS	N-CA-C	-8.54	103.30	114.31
4	D	115	THR	CA-C-N	6.79	126.71	119.85
4	D	115	THR	C-N-CA	6.79	126.71	119.85
4	D	118	ILE	CB-CA-C	6.78	120.34	111.53
2	B	71	THR	CA-C-N	6.46	126.22	119.76
2	B	71	THR	C-N-CA	6.46	126.22	119.76
1	A	231	VAL	CB-CA-C	-6.24	104.73	111.59
1	A	42	SER	N-CA-C	6.20	118.12	111.36
1	A	268	LYS	CA-C-N	6.18	127.56	119.84
1	A	268	LYS	C-N-CA	6.18	127.56	119.84
5	E	26	ASP	N-CA-CB	-5.80	103.32	110.98
5	E	208	ASN	N-CA-C	5.66	117.91	109.25
1	A	11	SER	CA-C-N	-5.55	115.88	123.14
1	A	11	SER	C-N-CA	-5.55	115.88	123.14
4	D	172	ASP	N-CA-C	-5.54	104.09	111.02
2	B	6	LYS	N-CA-C	-5.42	100.86	109.96
5	E	100	GLY	N-CA-C	5.33	125.81	113.18
5	E	41	MET	N-CA-C	5.33	117.27	110.61
1	A	270	LEU	N-CA-C	5.21	117.98	110.28
4	D	84	ASP	N-CA-C	-5.19	106.63	113.17
4	D	41	LYS	N-CA-C	5.17	115.11	108.34
2	B	85	VAL	CB-CA-C	-5.08	102.08	111.79
5	E	14	LYS	N-CA-C	-5.08	103.01	110.52
1	A	244	TRP	N-CA-C	5.00	117.73	109.72

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	E	25	GLN	Peptide
5	E	99	ALA	Peptide

5.2 Too-close contacts ⓘ

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	2247	0	2096	17	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	843	0	811	6	0
3	C	75	0	72	1	0
4	D	1552	0	1461	13	0
5	E	1927	0	1830	13	0
6	A	30	0	40	0	0
6	E	12	0	16	1	0
7	B	5	0	0	0	0
8	A	19	0	0	0	0
8	B	16	0	0	0	0
8	D	7	0	0	0	0
8	E	24	0	0	0	0
All	All	6757	0	6326	47	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 4.

All (47) 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:162:ASP:OD2	4:D:162:ASP:N	2.30	0.63
5:E:95:ARG:HG2	5:E:106:GLN:HB2	1.84	0.59
1:A:25:VAL:HG13	1:A:32:GLN:HE21	1.68	0.57
1:A:188:HIS:HB3	1:A:204:TRP:HB2	1.88	0.55
4:D:118:ILE:HD11	4:D:145:ASP:HA	1.90	0.53
5:E:124:PRO:HD3	5:E:232:PRO:HB3	1.93	0.50
4:D:183:ASN:N	4:D:183:ASN:OD1	2.44	0.50
1:A:55:GLU:OE1	1:A:170:ARG:NH2	2.45	0.49
1:A:6:ARG:HD3	1:A:98:MET:HE3	1.92	0.49
1:A:5:MET:HB2	1:A:168:LEU:HD13	1.94	0.49
5:E:57:GLN:HB2	5:E:61:PRO:HB3	1.95	0.48
1:A:72:GLN:HG2	1:A:75:ARG:HH21	1.78	0.48
5:E:36:ARG:NH1	5:E:65:TYR:OH	2.45	0.48
1:A:154:GLU:OE1	5:E:102:ARG:NH1	2.47	0.48
5:E:38:ASP:HA	5:E:39:PRO:HD2	1.65	0.48
1:A:268:LYS:HA	1:A:269:PRO:HD2	1.69	0.47
2:B:55:SER:OG	2:B:56:PHE:N	2.48	0.47
4:D:186:ASP:N	4:D:186:ASP:OD1	2.48	0.46
2:B:48:LYS:O	2:B:68:THR:OG1	2.31	0.46
4:D:82:PRO:HA	4:D:114:VAL:HB	1.98	0.46
4:D:138:VAL:HG11	5:E:146:VAL:HG21	1.98	0.45
1:A:223:ASP:OD1	1:A:223:ASP:N	2.35	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:ASP:OD1	1:A:113:TYR:OH	2.23	0.45
1:A:159:TYR:OH	3:C:1:LEU:O	2.30	0.45
2:B:64:LEU:HD12	2:B:64:LEU:HA	1.80	0.45
5:E:209:HIS:ND1	6:E:248:GOL:H31	2.33	0.44
2:B:96:ASP:HB3	2:B:99:MET:HB2	1.98	0.44
5:E:177:GLN:HE21	5:E:177:GLN:HB2	1.56	0.44
4:D:171:MET:HB3	4:D:173:PHE:HB2	1.99	0.44
4:D:120:ASN:HA	4:D:121:PRO:HD2	1.53	0.44
4:D:32:PHE:HD1	4:D:92:VAL:HG22	1.83	0.44
1:A:47:PRO:O	1:A:48:ARG:NH1	2.45	0.43
1:A:156:LEU:HD23	1:A:156:LEU:HA	1.77	0.43
1:A:195:SER:O	1:A:197:HIS:N	2.51	0.43
1:A:196:ASP:OD1	1:A:196:ASP:N	2.50	0.43
4:D:6:ASN:HD22	4:D:6:ASN:HA	1.64	0.42
4:D:153:SER:OG	4:D:158:VAL:O	2.37	0.42
5:E:29:HIS:ND1	5:E:94:SER:OG	2.48	0.42
4:D:201:ASP:OD2	4:D:201:ASP:N	2.53	0.41
4:D:154:LYS:HB3	4:D:154:LYS:HE3	1.89	0.41
2:B:1:ILE:HD12	2:B:1:ILE:HA	1.61	0.41
5:E:231:LYS:HA	5:E:232:PRO:HD3	1.87	0.41
5:E:148:LEU:HD23	5:E:148:LEU:HA	1.80	0.41
1:A:48:ARG:HA	1:A:48:ARG:HD3	1.82	0.40
1:A:189:MET:HE3	1:A:274:TRP:HB2	2.03	0.40
5:E:59:GLU:H	5:E:59:GLU:HG3	1.69	0.40
2:B:71:THR:HA	2:B:72:PRO:HD2	1.88	0.40

There are no symmetry-related clashes.

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%)	265 (97%)	6 (2%)	2 (1%)	18 41

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	99/100 (99%)	98 (99%)	1 (1%)	0	100	100
3	C	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
4	D	198/200 (99%)	182 (92%)	15 (8%)	1 (0%)	24	48
5	E	243/245 (99%)	230 (95%)	11 (4%)	2 (1%)	16	37
All	All	820/829 (99%)	781 (95%)	34 (4%)	5 (1%)	21	44

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	196	ASP
4	D	6	ASN
5	E	39	PRO
5	E	183	PRO
1	A	269	PRO

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%)	209 (90%)	22 (10%)	8	20
2	B	96/95 (101%)	82 (85%)	14 (15%)	3	8
3	C	7/7 (100%)	4 (57%)	3 (43%)	0	0
4	D	178/178 (100%)	147 (83%)	31 (17%)	2	5
5	E	209/209 (100%)	174 (83%)	35 (17%)	2	6
All	All	721/720 (100%)	616 (85%)	105 (15%)	3	8

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	12	VAL
1	A	32	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	35	ARG
1	A	52	ILE
1	A	66	LYS
1	A	72	GLN
1	A	89	GLU
1	A	95	VAL
1	A	98	MET
1	A	115	GLN
1	A	146	LYS
1	A	182	THR
1	A	196	ASP
1	A	223	ASP
1	A	228	THR
1	A	247	VAL
1	A	249	VAL
1	A	253	GLN
1	A	256	ARG
1	A	262	GLN
1	A	272	LEU
2	B	0	MET
2	B	1	ILE
2	B	4	THR
2	B	6	LYS
2	B	44	GLU
2	B	50	GLU
2	B	64	LEU
2	B	68	THR
2	B	70	PHE
2	B	75	LYS
2	B	85	VAL
2	B	91	LYS
2	B	98	ASP
2	B	99	MET
3	C	1	LEU
3	C	6	VAL
3	C	7	ASN
4	D	1	LYS
4	D	6	ASN
4	D	12	VAL
4	D	23	THR
4	D	31	SER
4	D	41	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	51	SER
4	D	63	THR
4	D	73	VAL
4	D	76	LEU
4	D	87	THR
4	D	100	SER
4	D	103	LYS
4	D	110	THR
4	D	120	ASN
4	D	127	GLN
4	D	128	LEU
4	D	130	ASP
4	D	135	ASP
4	D	137	SER
4	D	138	VAL
4	D	151	SER
4	D	152	GLN
4	D	154	LYS
4	D	158	VAL
4	D	162	ASP
4	D	170	SER
4	D	183	ASN
4	D	186	ASP
4	D	195	ASN
4	D	197	ILE
5	E	7	THR
5	E	12	VAL
5	E	14	LYS
5	E	25	GLN
5	E	27	MET
5	E	55	THR
5	E	59	GLU
5	E	66	ASN
5	E	67	VAL
5	E	70	SER
5	E	72	THR
5	E	81	SER
5	E	88	SER
5	E	105	GLU
5	E	113	ARG
5	E	119	LEU
5	E	120	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	129	VAL
5	E	133	SER
5	E	137	ILE
5	E	138	SER
5	E	145	LEU
5	E	146	VAL
5	E	148	LEU
5	E	163	VAL
5	E	166	LYS
5	E	170	SER
5	E	172	VAL
5	E	177	GLN
5	E	182	GLN
5	E	187	ASP
5	E	192	LEU
5	E	195	ARG
5	E	226	THR
5	E	246	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	43	GLN
1	A	72	GLN
1	A	253	GLN
2	B	13	HIS
4	D	5	GLN
4	D	6	ASN
4	D	37	GLN
4	D	81	GLN
4	D	105	GLN
4	D	111	GLN
4	D	119	GLN
5	E	28	ASN
5	E	37	GLN
5	E	62	ASN
5	E	141	GLN
5	E	156	HIS

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 ⓘ

8 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	E	248	-	5,5,5	0.46	0	5,5,5	0.78	0
6	GOL	A	277	-	5,5,5	0.48	0	5,5,5	0.79	0
7	SO4	B	100	-	4,4,4	0.55	0	6,6,6	0.36	0
6	GOL	E	247	-	5,5,5	0.37	0	5,5,5	0.93	0
6	GOL	A	279	-	5,5,5	0.41	0	5,5,5	0.42	0
6	GOL	A	278	-	5,5,5	0.45	0	5,5,5	1.07	1 (20%)
6	GOL	A	280	-	5,5,5	0.44	0	5,5,5	0.56	0
6	GOL	A	276	-	5,5,5	0.64	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
6	GOL	E	248	-	-	0/4/4/4	-
6	GOL	A	277	-	-	2/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	E	247	-	-	2/4/4/4	-
6	GOL	A	279	-	-	2/4/4/4	-
6	GOL	A	278	-	-	3/4/4/4	-
6	GOL	A	280	-	-	0/4/4/4	-
6	GOL	A	276	-	-	2/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	278	GOL	O1-C1-C2	-2.04	101.19	110.38

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	276	GOL	O1-C1-C2-C3
6	A	277	GOL	O1-C1-C2-C3
6	A	278	GOL	O1-C1-C2-C3
6	A	279	GOL	C1-C2-C3-O3
6	E	247	GOL	O1-C1-C2-C3
6	A	276	GOL	O1-C1-C2-O2
6	A	279	GOL	O2-C2-C3-O3
6	A	277	GOL	O1-C1-C2-O2
6	A	278	GOL	O1-C1-C2-O2
6	E	247	GOL	O1-C1-C2-O2
6	A	278	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	248	GOL	1	0

5.7 Other polymers [i](#)

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 ⓘ

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%)	0.73	33 (12%) 9 7	42, 55, 65, 71	0
2	B	100/100 (100%)	0.57	4 (4%) 42 38	32, 54, 65, 83	1 (1%)
3	C	9/9 (100%)	0.27	0 100 100	51, 56, 63, 63	0
4	D	200/200 (100%)	0.70	13 (6%) 25 22	42, 54, 66, 72	0
5	E	245/245 (100%)	0.43	8 (3%) 49 45	43, 54, 66, 72	0
All	All	829/829 (100%)	0.61	58 (6%) 22 19	32, 54, 66, 83	1 (0%)

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	223	ASP	4.2
1	A	197	HIS	4.2
1	A	199	ALA	4.1
1	A	251	SER	3.9
4	D	133	SER	3.8
1	A	257	TYR	3.7
1	A	254	GLU	3.7
1	A	259	CYS	3.7
1	A	200	THR	3.6
1	A	191	HIS	3.5
1	A	248	VAL	3.4
1	A	201	LEU	3.4
1	A	218	GLN	3.4
5	E	245	ALA	3.3
1	A	58	GLU	3.3
1	A	217	TRP	3.2
1	A	272	LEU	3.2
1	A	252	GLY	3.1
4	D	132	LYS	3.0
4	D	154	LYS	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	195	SER	2.9
4	D	185	SER	2.9
1	A	219	ARG	2.9
4	D	186	ASP	2.9
4	D	145	ASP	2.8
2	B	1	ILE	2.8
5	E	185	LEU	2.8
4	D	134	SER	2.8
1	A	253	GLN	2.7
1	A	256	ARG	2.7
1	A	216	THR	2.7
1	A	221	GLY	2.6
4	D	171	MET	2.6
5	E	184	ALA	2.6
1	A	247	VAL	2.5
5	E	226	THR	2.5
1	A	274	TRP	2.5
1	A	192	HIS	2.5
1	A	220	ASP	2.4
1	A	224	GLN	2.4
2	B	0	MET	2.4
2	B	99	MET	2.4
1	A	250	PRO	2.3
1	A	255	GLN	2.3
5	E	171	GLY	2.3
5	E	221	GLU	2.3
1	A	196	ASP	2.3
4	D	135	ASP	2.3
5	E	2	ALA	2.2
4	D	159	TYR	2.2
4	D	156	SER	2.2
1	A	145	HIS	2.2
2	B	16	GLU	2.1
5	E	117	GLU	2.1
4	D	153	SER	2.1
1	A	258	THR	2.1
4	D	189	CYS	2.0
1	A	245	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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	A	276	6/6	0.60	0.17	58,59,61,61	0
6	GOL	A	279	6/6	0.71	0.17	77,79,80,80	0
6	GOL	A	280	6/6	0.72	0.18	80,80,80,81	0
6	GOL	A	277	6/6	0.76	0.21	73,74,74,75	0
6	GOL	E	247	6/6	0.81	0.14	62,64,65,65	0
6	GOL	E	248	6/6	0.81	0.27	63,64,64,65	6
6	GOL	A	278	6/6	0.86	0.16	62,62,63,64	0
7	SO4	B	100	5/5	0.89	0.17	73,73,74,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.