



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:59 AM UTC

PDB ID : 2GJ6 / pdb_00002gj6
Title : The complex between TCR A6 and human Class I MHC HLA-A2 with the modified HTLV-1 TAX (Y5K-4-[3-Indolyl]-butyric acid) peptide
Authors : Borbulevych, O.Y.; Baker, B.M.
Deposited on : 2006-03-30
Resolution : 2.56 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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

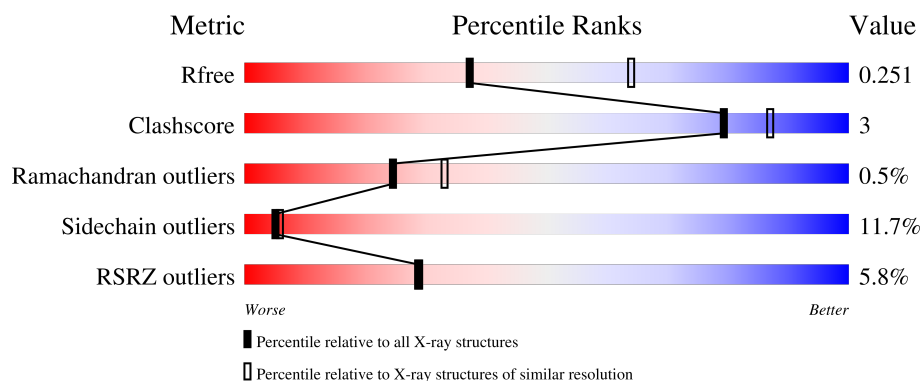
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 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	1853 (2.58-2.54)
Clashscore	190562	1897 (2.58-2.54)
Ramachandran outliers	187476	1875 (2.58-2.54)
Sidechain outliers	187428	1875 (2.58-2.54)
RSRZ outliers	180081	1853 (2.58-2.54)

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	7% 85% 12% .
2	B	100	2% 79% 16% 5%
3	C	9	89% 11%
4	D	200	12% 82% 16% .
5	E	245	2% 82% 13% ..

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6831 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, Contains: Beta-2-microglobulin variant pI 5.3.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	cloning artifact	UNP P61769

- Molecule 3 is a protein called Modified HTLV-1 TAX (Y5K-IBA) peptide, chain C.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			74	53	10	11			

- Molecule 4 is a protein called A6-Tcr.

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

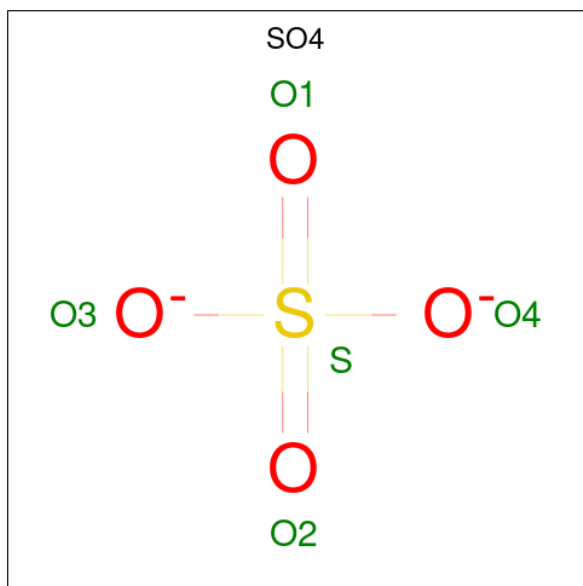
- Molecule 5 is a protein called A6-Tcr.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	243	Total	C	N	O	S	0	0	0
			1915	1202	336	369	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	1	ASN	-	cloning artifact	GB 6730544
E	2	ALA	-	cloning artifact	GB 6730544

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



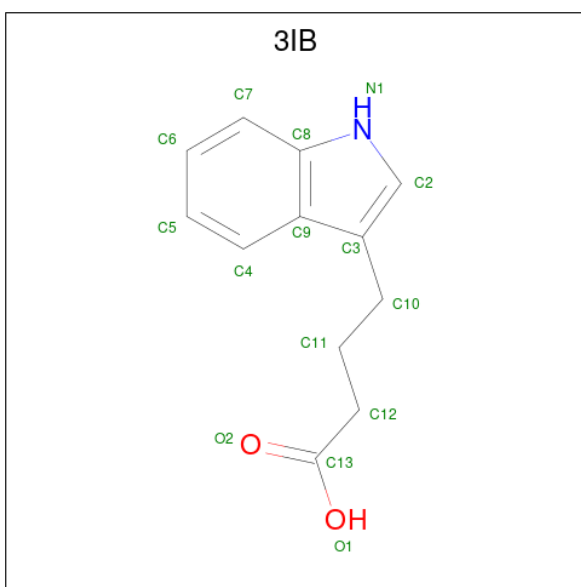
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	E	1	Total O S 5 4 1	0	0
6	E	1	Total O S 5 4 1	0	0

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 8 is 3-INDOLEBUTYRIC ACID (CCD ID: 3IB) (formula: C₁₂H₁₃NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	C	1	Total	C	N	O	0	0
			14	12	1	1		

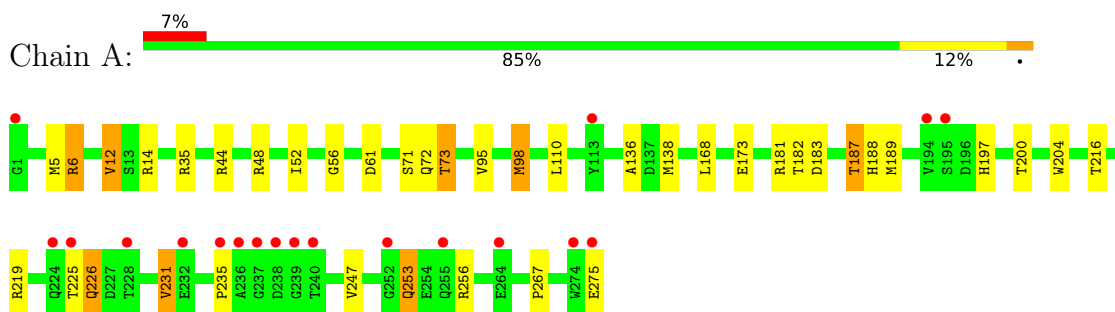
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	39	Total	O	0	0
			39	39		
9	B	19	Total	O	0	0
			19	19		
9	C	1	Total	O	0	0
			1	1		
9	D	14	Total	O	0	0
			14	14		
9	E	16	Total	O	0	0
			16	16		

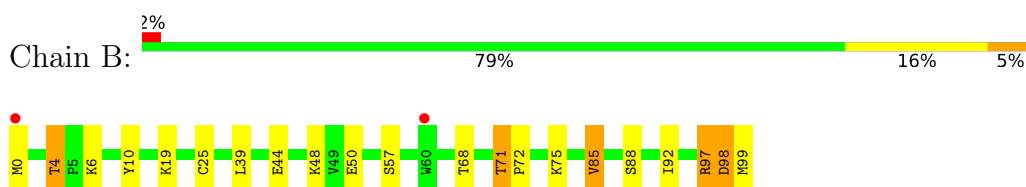
3 Residue-property plots

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.

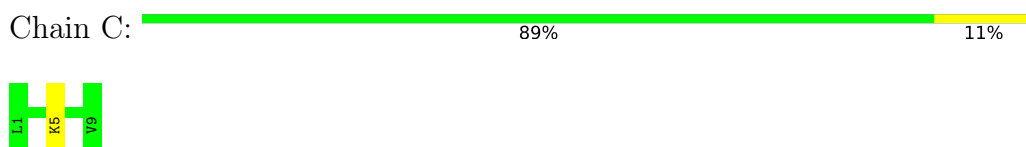
- Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



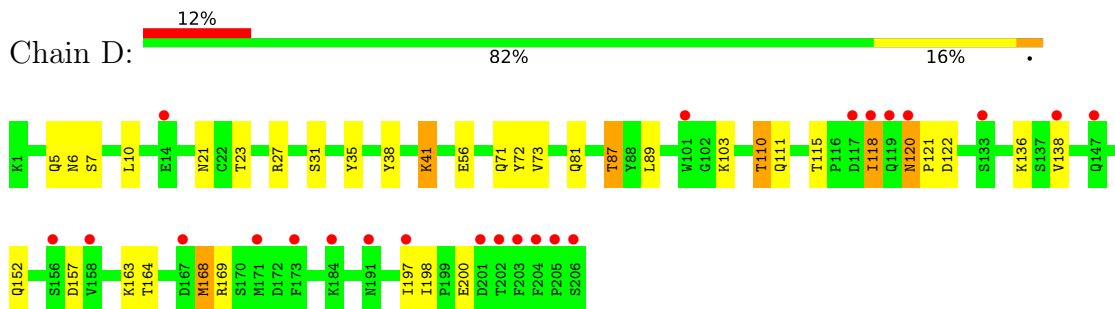
- Molecule 2: Beta-2-microglobulin, Contains: Beta-2-microglobulin variant pI 5.3



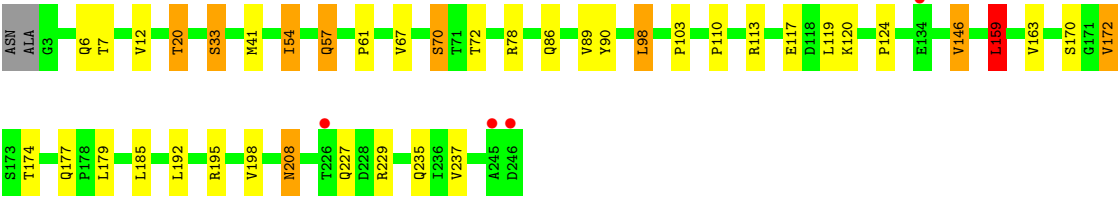
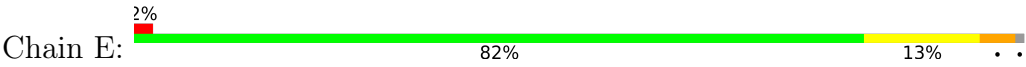
- Molecule 3: Modified HTLV-1 TAX (Y5K-IBA) peptide, chain C



- Molecule 4: A6-Tcr



- Molecule 5: A6-Tcr



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	223.85Å 49.02Å 94.17Å 90.00° 90.34° 90.00°	Depositor
Resolution (Å)	20.00 – 2.56 20.00 – 2.56	Depositor EDS
% Data completeness (in resolution range)	95.7 (20.00-2.56) 95.4 (20.00-2.56)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.23 (at 2.56Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.199 , 0.250 0.203 , 0.251	Depositor DCC
R_{free} test set	1600 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	45.9	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 56.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.010 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6831	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% 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: GOL, SO4, 3IB

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	0.93	7/2312 (0.3%)	1.11	6/3137 (0.2%)
2	B	0.81	0/860	1.09	5/1162 (0.4%)
3	C	0.89	0/76	1.45	0/101
4	D	0.75	2/1585 (0.1%)	1.04	4/2150 (0.2%)
5	E	0.76	0/1968	1.07	8/2681 (0.3%)
All	All	0.83	9/6801 (0.1%)	1.08	23/9231 (0.2%)

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
1	A	0	2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	197	HIS	CE1-NE2	11.58	1.44	1.32
1	A	197	HIS	CG-CD2	9.26	1.46	1.35
1	A	253	GLN	CD-OE1	8.18	1.39	1.23
4	D	120	ASN	CG-ND2	7.37	1.48	1.33
1	A	226	GLN	CD-NE2	7.35	1.48	1.33
1	A	197	HIS	CG-ND1	7.25	1.46	1.38
1	A	12	VAL	CA-CB	6.27	1.62	1.54
1	A	253	GLN	CD-NE2	5.61	1.45	1.33
4	D	118	ILE	C-O	5.08	1.29	1.24

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	120	ASN	OD1-CG-ND2	8.54	131.14	122.60
1	A	231	VAL	CB-CA-C	-6.44	104.50	111.59
2	B	71	THR	CA-C-N	6.29	126.23	119.76
2	B	71	THR	C-N-CA	6.29	126.23	119.76
2	B	85	VAL	CB-CA-C	-6.17	103.04	112.05
5	E	124	PRO	CA-C-N	-6.00	113.78	120.14
5	E	124	PRO	C-N-CA	-6.00	113.78	120.14
2	B	6	LYS	N-CA-C	-5.94	100.88	110.32
5	E	172	VAL	N-CA-C	5.90	117.07	108.58
1	A	73	THR	N-CA-CB	5.78	118.39	110.01
5	E	33	SER	N-CA-C	5.76	117.94	109.24
5	E	54	ILE	N-CA-CB	-5.57	104.25	111.82
5	E	159	LEU	CA-CB-CG	5.45	135.38	116.30
4	D	120	ASN	CB-CG-ND2	-5.41	108.28	116.40
4	D	122	ASP	CA-C-N	5.32	125.24	119.76
4	D	122	ASP	C-N-CA	5.32	125.24	119.76
1	A	136	ALA	N-CA-C	5.30	117.14	111.36
5	E	57	GLN	N-CA-C	5.17	118.53	110.32
2	B	4	THR	CB-CA-C	-5.16	101.36	109.11
5	E	208	ASN	N-CA-C	5.16	118.03	109.46
1	A	182	THR	CB-CA-C	5.13	118.35	110.14
1	A	56	GLY	CA-C-N	5.12	124.91	119.28
1	A	56	GLY	C-N-CA	5.12	124.91	119.28

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	187	THR	Peptide
1	A	253	GLN	Sidechain

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	7	0
2	B	837	0	803	7	0
3	C	74	0	81	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1552	0	1461	10	0
5	E	1915	0	1818	15	0
6	A	10	0	0	0	0
6	B	5	0	0	0	0
6	E	10	0	0	1	0
7	A	12	0	16	0	0
7	B	48	0	64	1	0
7	C	6	0	8	0	0
7	E	12	0	16	1	0
8	C	14	0	12	1	0
9	A	39	0	0	0	0
9	B	19	0	0	1	0
9	C	1	0	0	0	0
9	D	14	0	0	0	0
9	E	16	0	0	0	0
All	All	6831	0	6375	36	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 3.

All (36) 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:164:THR:OG1	5:E:195:ARG:NH1	2.23	0.70
4:D:21:ASN:ND2	4:D:72:TYR:OH	2.31	0.64
4:D:38:TYR:HB2	4:D:41:LYS:HD2	1.80	0.62
5:E:159:LEU:HD23	5:E:192:LEU:HD23	1.91	0.51
1:A:6:ARG:HB3	1:A:98:MET:HE3	1.95	0.49
1:A:5:MET:HB2	1:A:168:LEU:HD13	1.95	0.48
1:A:235:PRO:O	2:B:10:TYR:OH	2.29	0.48
2:B:25:CYS:HB2	2:B:39:LEU:HD21	1.96	0.48
5:E:70:SER:OG	6:E:414:SO4:O1	2.32	0.47
2:B:98:ASP:N	2:B:98:ASP:OD1	2.45	0.47
1:A:73:THR:HG22	5:E:98:LEU:HG	1.97	0.47
4:D:120:ASN:HA	4:D:121:PRO:HD3	1.65	0.46
4:D:169:ARG:NH1	5:E:170:SER:OG	2.49	0.45
5:E:120:LYS:HD2	5:E:227:GLN:HB2	1.98	0.45
4:D:87:THR:HA	4:D:111:GLN:HA	1.98	0.45
4:D:38:TYR:HB2	4:D:41:LYS:CD	2.45	0.44
5:E:89:VAL:HG22	5:E:113:ARG:HG2	1.99	0.44
5:E:57:GLN:HB2	5:E:61:PRO:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:48:LYS:O	2:B:68:THR:HG23	2.17	0.44
5:E:227:GLN:HG3	5:E:229:ARG:H	1.83	0.44
7:B:411:GOL:H12	9:B:429:HOH:O	2.18	0.44
4:D:35:TYR:HB2	4:D:89:LEU:HB2	1.98	0.44
5:E:146:VAL:HG12	5:E:195:ARG:HG3	2.00	0.44
1:A:188:HIS:HB3	1:A:204:TRP:HB2	2.01	0.43
5:E:6:GLN:HG2	5:E:110:PRO:HD2	2.00	0.42
4:D:41:LYS:HE2	4:D:41:LYS:HB2	1.90	0.42
2:B:71:THR:HA	2:B:72:PRO:HD2	1.78	0.42
5:E:86:GLN:O	5:E:90:TYR:OH	2.34	0.42
2:B:97:ARG:H	2:B:97:ARG:HG2	1.57	0.41
8:C:10:3IB:H2	5:E:103:PRO:O	2.19	0.41
4:D:5:GLN:HE21	4:D:110:THR:HG22	1.86	0.41
5:E:20:THR:HB	5:E:78:ARG:HG2	2.03	0.41
1:A:44:ARG:NH2	1:A:61:ASP:OD1	2.54	0.41
5:E:174:THR:HG21	7:E:410:GOL:H31	2.03	0.40
1:A:48:ARG:HD3	1:A:48:ARG:HA	1.70	0.40
2:B:99:MET:HE3	2:B:99:MET:HB3	1.85	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	273/275 (99%)	259 (95%)	13 (5%)	1 (0%)	30	39
2	B	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
3	C	7/9 (78%)	7 (100%)	0	0	100	100
4	D	198/200 (99%)	175 (88%)	20 (10%)	3 (2%)	8	10
5	E	241/245 (98%)	228 (95%)	13 (5%)	0	100	100
All	All	817/829 (99%)	764 (94%)	49 (6%)	4 (0%)	24	33

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	7	SER
4	D	6	ASN
4	D	168	MET
1	A	267	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%)	206 (89%)	25 (11%)	6	7
2	B	95/95 (100%)	83 (87%)	12 (13%)	4	4
3	C	8/8 (100%)	7 (88%)	1 (12%)	4	4
4	D	178/178 (100%)	155 (87%)	23 (13%)	4	4
5	E	208/209 (100%)	185 (89%)	23 (11%)	6	6
All	All	720/721 (100%)	636 (88%)	84 (12%)	5	6

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ARG
1	A	12	VAL
1	A	14	ARG
1	A	35	ARG
1	A	52	ILE
1	A	71	SER
1	A	72	GLN
1	A	95	VAL
1	A	98	MET
1	A	110	LEU
1	A	138	MET
1	A	173	GLU
1	A	181	ARG
1	A	183	ASP

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Mol	Chain	Res	Type
1	A	187	THR
1	A	189	MET
1	A	200	THR
1	A	216	THR
1	A	219	ARG
1	A	225	THR
1	A	226	GLN
1	A	231	VAL
1	A	247	VAL
1	A	256	ARG
1	A	275	GLU
2	B	0	MET
2	B	4	THR
2	B	19	LYS
2	B	44	GLU
2	B	50	GLU
2	B	57	SER
2	B	75	LYS
2	B	85	VAL
2	B	88	SER
2	B	92	ILE
2	B	97	ARG
2	B	98	ASP
3	C	5	LYS
4	D	10	LEU
4	D	23	THR
4	D	27	ARG
4	D	31	SER
4	D	41	LYS
4	D	56	GLU
4	D	71	GLN
4	D	73	VAL
4	D	81	GLN
4	D	87	THR
4	D	103	LYS
4	D	110	THR
4	D	115	THR
4	D	118	ILE
4	D	136	LYS
4	D	138	VAL
4	D	152	GLN
4	D	157	ASP

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Mol	Chain	Res	Type
4	D	163	LYS
4	D	168	MET
4	D	197	ILE
4	D	198	ILE
4	D	200	GLU
5	E	7	THR
5	E	12	VAL
5	E	20	THR
5	E	33	SER
5	E	41	MET
5	E	54	ILE
5	E	67	VAL
5	E	70	SER
5	E	72	THR
5	E	98	LEU
5	E	117	GLU
5	E	119	LEU
5	E	146	VAL
5	E	159	LEU
5	E	163	VAL
5	E	172	VAL
5	E	177	GLN
5	E	179	LEU
5	E	185	LEU
5	E	198	VAL
5	E	208	ASN
5	E	235	GLN
5	E	237	VAL

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	86	ASN
1	A	224	GLN
1	A	253	GLN
2	B	83	ASN
4	D	6	ASN
4	D	21	ASN
4	D	37	GLN
4	D	65	GLN
4	D	105	GLN
4	D	111	GLN

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Mol	Chain	Res	Type
4	D	149	ASN
4	D	191	ASN
5	E	17	GLN
5	E	37	GLN
5	E	57	GLN
5	E	121	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 ⓘ

19 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	$\# Z > 2$
7	GOL	A	413	-	5,5,5	0.30	0	5,5,5	0.58	0
7	GOL	B	401	-	5,5,5	0.33	0	5,5,5	0.67	0
7	GOL	C	405	-	5,5,5	0.39	0	5,5,5	0.54	0
7	GOL	B	403	-	5,5,5	0.45	0	5,5,5	0.94	0
6	SO4	B	417	-	4,4,4	0.27	0	6,6,6	0.17	0
8	3IB	C	10	3	15,15,16	1.71	4 (26%)	19,19,21	1.48	3 (15%)
7	GOL	B	408	-	5,5,5	0.47	0	5,5,5	1.20	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	GOL	E	404	-	5,5,5	0.43	0	5,5,5	0.49	0
6	SO4	E	414	-	4,4,4	0.16	0	6,6,6	0.39	0
6	SO4	E	415	-	4,4,4	0.30	0	6,6,6	0.34	0
7	GOL	B	407	-	5,5,5	0.51	0	5,5,5	0.51	0
7	GOL	B	412	-	5,5,5	0.38	0	5,5,5	0.80	0
6	SO4	A	418	-	4,4,4	0.24	0	6,6,6	0.34	0
7	GOL	E	410	-	5,5,5	0.33	0	5,5,5	0.56	0
7	GOL	A	402	-	5,5,5	0.60	0	5,5,5	1.95	2 (40%)
6	SO4	A	416	-	4,4,4	0.26	0	6,6,6	0.26	0
7	GOL	B	409	-	5,5,5	0.37	0	5,5,5	1.01	0
7	GOL	B	411	-	5,5,5	0.33	0	5,5,5	1.19	0
7	GOL	B	406	-	5,5,5	0.34	0	5,5,5	0.71	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
7	GOL	A	413	-	-	3/4/4/4	-
8	3IB	C	10	3	-	0/5/5/6	0/2/2/2
7	GOL	B	409	-	-	4/4/4/4	-
7	GOL	B	408	-	-	4/4/4/4	-
7	GOL	B	401	-	-	3/4/4/4	-
7	GOL	B	407	-	-	2/4/4/4	-
7	GOL	B	411	-	-	0/4/4/4	-
7	GOL	B	412	-	-	2/4/4/4	-
7	GOL	E	410	-	-	4/4/4/4	-
7	GOL	B	406	-	-	0/4/4/4	-
7	GOL	A	402	-	-	2/4/4/4	-
7	GOL	C	405	-	-	4/4/4/4	-
7	GOL	B	403	-	-	2/4/4/4	-
7	GOL	E	404	-	-	4/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	10	3IB	O1-C13	-4.09	1.21	1.42
8	C	10	3IB	C9-C3	2.91	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	10	3IB	C8-N1	-2.45	1.33	1.37
8	C	10	3IB	C9-C8	-2.45	1.38	1.41

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	402	GOL	O3-C3-C2	-3.29	95.57	110.38
8	C	10	3IB	C4-C9-C8	3.20	122.16	118.84
8	C	10	3IB	C7-C8-C9	-2.50	119.77	122.19
8	C	10	3IB	C8-N1-C2	2.45	111.26	109.08
7	A	402	GOL	C3-C2-C1	-2.10	104.11	111.80
7	B	408	GOL	O1-C1-C2	-2.08	101.01	110.38

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	402	GOL	O1-C1-C2-C3
7	A	413	GOL	C1-C2-C3-O3
7	B	407	GOL	O1-C1-C2-C3
7	B	408	GOL	O1-C1-C2-C3
7	B	408	GOL	C1-C2-C3-O3
7	B	409	GOL	O1-C1-C2-C3
7	B	409	GOL	C1-C2-C3-O3
7	B	412	GOL	O1-C1-C2-C3
7	C	405	GOL	O1-C1-C2-C3
7	C	405	GOL	C1-C2-C3-O3
7	E	404	GOL	O1-C1-C2-C3
7	E	404	GOL	C1-C2-C3-O3
7	E	410	GOL	O1-C1-C2-O2
7	E	410	GOL	O1-C1-C2-C3
7	E	410	GOL	C1-C2-C3-O3
7	B	401	GOL	C1-C2-C3-O3
7	B	403	GOL	O1-C1-C2-C3
7	A	413	GOL	O2-C2-C3-O3
7	B	403	GOL	O1-C1-C2-O2
7	B	407	GOL	O1-C1-C2-O2
7	B	408	GOL	O2-C2-C3-O3
7	C	405	GOL	O1-C1-C2-O2
7	C	405	GOL	O2-C2-C3-O3
7	E	404	GOL	O1-C1-C2-O2
7	B	409	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
7	B	409	GOL	O2-C2-C3-O3
7	E	404	GOL	O2-C2-C3-O3
7	A	402	GOL	C1-C2-C3-O3
7	A	413	GOL	O1-C1-C2-O2
7	B	408	GOL	O1-C1-C2-O2
7	B	412	GOL	O1-C1-C2-O2
7	B	401	GOL	O1-C1-C2-O2
7	B	401	GOL	O2-C2-C3-O3
7	E	410	GOL	O2-C2-C3-O3

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	10	3IB	1	0
6	E	414	SO4	1	0
7	E	410	GOL	1	0
7	B	411	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%)	0.47	19 (6%) 23 22	36, 45, 53, 58	0
2	B	100/100 (100%)	0.27	2 (2%) 65 65	36, 45, 54, 62	0
3	C	9/9 (100%)	-0.20	0 100 100	39, 43, 45, 46	0
4	D	200/200 (100%)	0.87	23 (11%) 9 9	32, 43, 50, 66	0
5	E	243/245 (99%)	0.29	4 (1%) 70 72	26, 44, 53, 56	0
All	All	827/829 (99%)	0.48	48 (5%) 29 29	26, 44, 53, 66	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	206	SER	7.0
5	E	246	ASP	5.8
1	A	237	GLY	5.6
4	D	201	ASP	5.5
4	D	204	PHE	5.3
4	D	205	PRO	5.3
4	D	203	PHE	5.0
4	D	202	THR	4.1
1	A	236	ALA	3.9
1	A	235	PRO	3.9
4	D	117	ASP	3.7
4	D	197	ILE	3.6
5	E	245	ALA	3.5
4	D	119	GLN	3.4
1	A	239	GLY	3.2
1	A	1	GLY	3.1
4	D	118	ILE	3.1
1	A	275	GLU	3.1
4	D	171	MET	3.0
4	D	147	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
4	D	120	ASN	2.8
1	A	225	THR	2.8
1	A	195	SER	2.7
4	D	133	SER	2.7
1	A	264	GLU	2.6
1	A	228	THR	2.6
1	A	240	THR	2.5
4	D	184	LYS	2.5
5	E	134	GLU	2.5
2	B	0	MET	2.5
4	D	191	ASN	2.4
4	D	173	PHE	2.4
1	A	113	TYR	2.3
1	A	232	GLU	2.3
4	D	14	GLU	2.3
4	D	158	VAL	2.2
1	A	194	VAL	2.2
5	E	226	THR	2.2
2	B	60	TRP	2.2
4	D	138	VAL	2.2
1	A	224	GLN	2.2
4	D	156	SER	2.2
4	D	101	TRP	2.2
1	A	255	GLN	2.1
1	A	238	ASP	2.1
1	A	274	TRP	2.0
4	D	167	ASP	2.0
1	A	252	GLY	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(Å ²)	Q<0.9
7	GOL	E	410	6/6	0.60	0.25	42,44,44,47	6
7	GOL	B	412	6/6	0.75	0.23	31,37,37,40	6
6	SO4	A	418	5/5	0.75	0.18	44,44,45,46	5
7	GOL	C	405	6/6	0.77	0.21	33,38,38,39	6
7	GOL	B	407	6/6	0.78	0.25	38,40,41,42	6
7	GOL	A	413	6/6	0.81	0.16	45,46,47,49	6
7	GOL	B	401	6/6	0.81	0.19	37,38,39,40	6
7	GOL	B	408	6/6	0.84	0.21	54,55,57,57	0
7	GOL	E	404	6/6	0.85	0.13	40,42,43,43	6
7	GOL	B	409	6/6	0.85	0.14	46,48,48,49	6
7	GOL	B	403	6/6	0.86	0.17	57,60,61,63	0
7	GOL	B	411	6/6	0.86	0.17	50,54,56,62	0
7	GOL	B	406	6/6	0.86	0.12	38,40,40,40	6
6	SO4	B	417	5/5	0.91	0.14	42,42,44,44	5
6	SO4	A	416	5/5	0.92	0.14	40,41,42,42	5
6	SO4	E	415	5/5	0.93	0.13	37,38,39,39	5
7	GOL	A	402	6/6	0.93	0.10	30,40,42,45	0
8	3IB	C	10	14/15	0.96	0.10	30,32,35,38	0
6	SO4	E	414	5/5	0.97	0.17	48,48,49,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.