



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:50 PM UTC

PDB ID : 6PY2 / pdb_00006py2
Title : HLA-TCR complex
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Deposited on : 2019-07-28
Resolution : 2.83 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)
Xtrriage (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

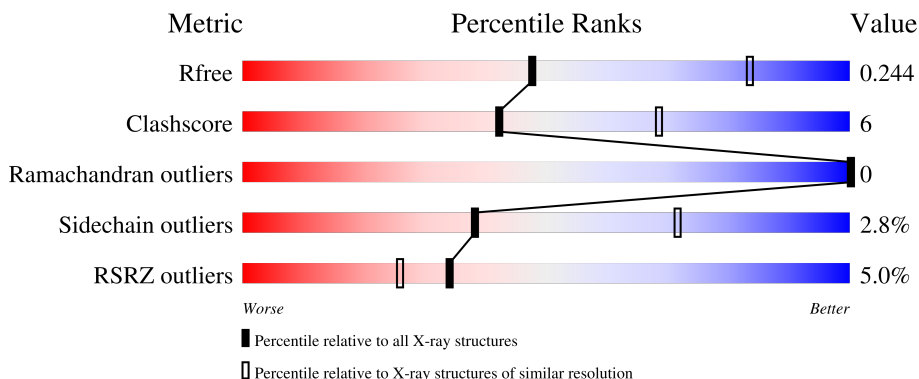
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.83 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	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

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	254	 1% (upper red bar), 8% (red), 61% (green), 10% (yellow), 21% (grey)
2	B	261	 3% (upper red bar), 3% (red), 53% (green), 14% (yellow), 30% (grey)
3	C	12	 8% (red), 83% (green), 9% (yellow)
4	D	206	 9% (upper red bar), 9% (red), 77% (green), 15% (yellow), 1% (grey)
5	E	245	 4% (upper red bar), 4% (red), 83% (green), 13% (yellow), 1% (grey)

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6457 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 II histocompatibility antigen DQ alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	182	1461	947	234	278	2	0	0	0

- Molecule 2 is a protein called HLA class II histocompatibility antigen DQ beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	178	1458	922	260	269	7	0	0	0

- Molecule 3 is a protein called DQ2.2-glut-L1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	12	91	58	14	19	0	0	0

- Molecule 4 is a protein called T-cell receptor, T594, alpha chain,T-cell receptor, T594, alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	191	1463	920	234	301	8	0	0	0

- Molecule 5 is a protein called T-cell receptor, T594, beta chain,T-cell receptor, T594, beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	243	1909	1211	332	361	5	0	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		

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



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

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

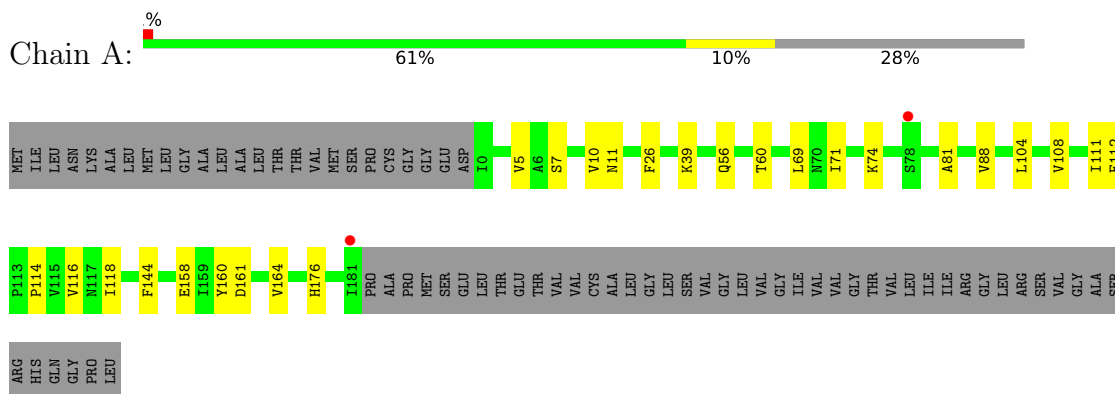
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	7	Total	O	0	0
			7	7		
8	B	3	Total	O	0	0
			3	3		
8	D	6	Total	O	0	0
			6	6		
8	E	5	Total	O	0	0
			5	5		

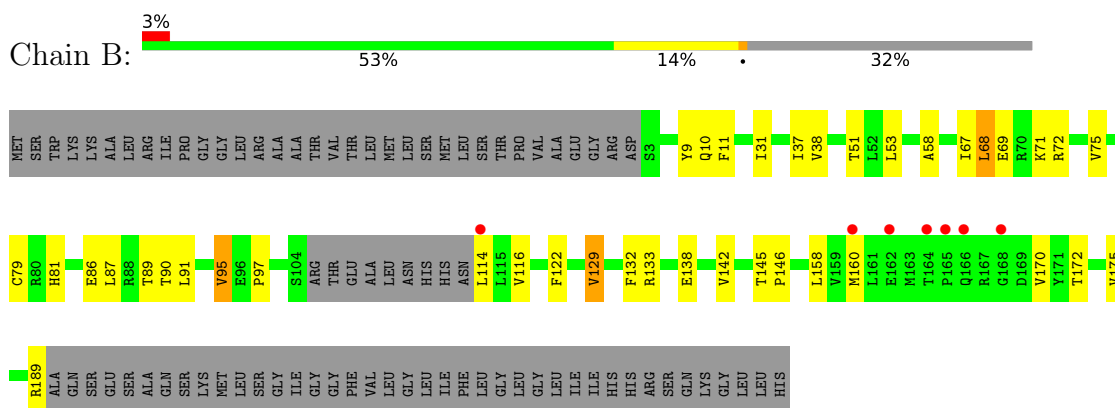
3 Residue-property plots [i](#)

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.

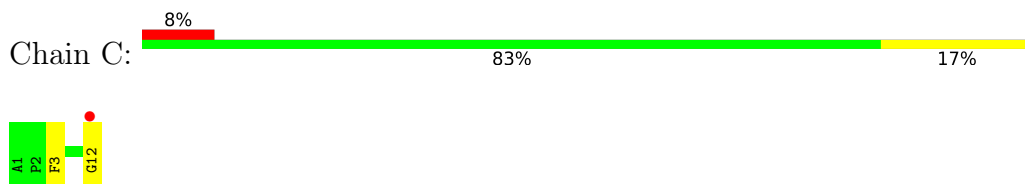
- Molecule 1: HLA class II histocompatibility antigen DQ alpha chain



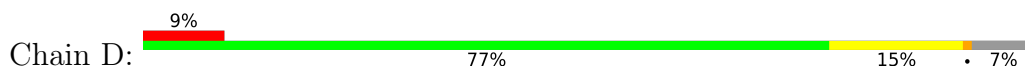
- Molecule 2: HLA class II histocompatibility antigen DQ beta chain

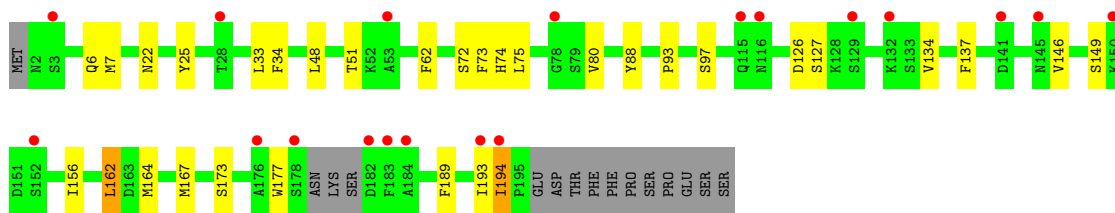


- Molecule 3: DQ2.2-glut-L1

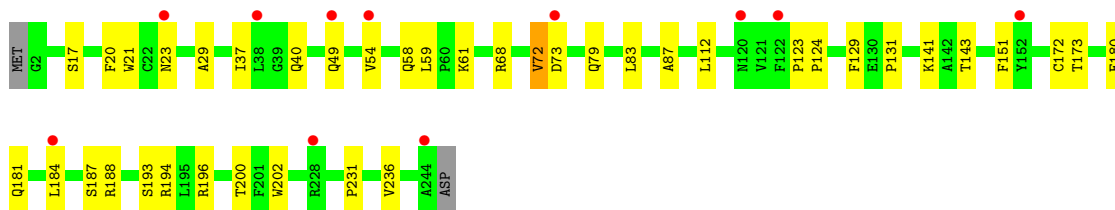
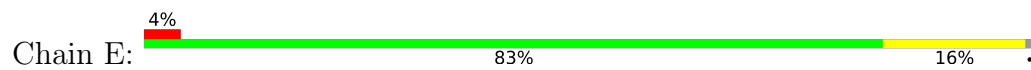


- Molecule 4: T-cell receptor, T594, alpha chain, T-cell receptor, T594, alpha chain





- Molecule 5: T-cell receptor, T594, beta chain, T-cell receptor, T594, beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	75.28Å 275.14Å 141.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.86 – 2.83 45.86 – 2.83	Depositor EDS
% Data completeness (in resolution range)	85.0 (45.86-2.83) 85.0 (45.86-2.83)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.07 (at 2.81Å)	Xtrriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.216 , 0.244 0.217 , 0.244	Depositor DCC
R_{free} test set	1570 reflections (4.39%)	wwPDB-VP
Wilson B-factor (Å ²)	62.1	Xtrriage
Anisotropy	0.024	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 43.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6457	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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: GOL, NAG

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	0.17	0/1505	0.32	0/2057
2	B	0.16	0/1491	0.38	0/2026
3	C	0.11	0/93	0.26	0/126
4	D	0.13	0/1494	0.33	0/2029
5	E	0.15	0/1961	0.36	0/2671
All	All	0.15	0/6544	0.35	0/8909

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	1461	0	1402	20	0
2	B	1458	0	1423	26	0
3	C	91	0	86	2	0
4	D	1463	0	1374	20	0
5	E	1909	0	1826	24	0
6	A	28	0	26	0	0
6	B	14	0	13	0	0
7	A	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	E	6	0	8	0	0
8	A	7	0	0	0	0
8	B	3	0	0	0	0
8	D	6	0	0	0	0
8	E	5	0	0	0	0
All	All	6457	0	6166	79	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 6.

All (79) 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:167:MET:HE1	5:E:141:LYS:HZ1	1.18	1.03
4:D:167:MET:HE1	5:E:141:LYS:NZ	1.91	0.85
1:A:60:THR:HG21	5:E:49:GLN:HG3	1.62	0.79
1:A:56:GLN:HB3	5:E:49:GLN:HG2	1.71	0.71
5:E:49:GLN:HB2	5:E:54:VAL:CG2	2.22	0.69
2:B:114:LEU:HD11	2:B:160:MET:HB3	1.74	0.69
4:D:7:MET:HE3	4:D:22:ASN:H	1.59	0.68
4:D:162:LEU:HB3	5:E:172:CYS:HB2	1.79	0.64
4:D:6:GLN:NE2	4:D:88:TYR:O	2.33	0.62
5:E:20:PHE:HZ	5:E:112:LEU:HD22	1.65	0.61
1:A:88:VAL:HG22	1:A:108:VAL:HG12	1.83	0.60
1:A:161:ASP:OD1	1:A:176:HIS:ND1	2.35	0.59
1:A:108:VAL:HG23	1:A:111:ILE:HD11	1.85	0.58
4:D:62:PHE:HB3	4:D:75:LEU:HD11	1.85	0.58
1:A:158:GLU:HG2	1:A:160:TYR:CZ	2.40	0.57
1:A:69:LEU:HD13	2:B:9:TYR:HB2	1.86	0.56
5:E:37:ILE:HG12	5:E:87:ALA:HB2	1.87	0.55
5:E:72:VAL:HG13	5:E:73:ASP:H	1.71	0.55
4:D:149:SER:HB2	4:D:156:ILE:HD11	1.89	0.55
5:E:184:LEU:HB2	5:E:187:SER:HB2	1.87	0.55
2:B:51:THR:HG22	2:B:53:LEU:H	1.73	0.54
1:A:81:ALA:HB1	1:A:112:PHE:HE1	1.74	0.53
2:B:145:THR:HG23	2:B:146:PRO:O	2.08	0.53
4:D:137:PHE:HB2	4:D:189:PHE:CE1	2.44	0.53
2:B:129:VAL:HB	2:B:175:VAL:HG22	1.91	0.52
4:D:34:PHE:HE2	4:D:93:PRO:HD3	1.74	0.52
1:A:114:PRO:HG3	1:A:144:PHE:CE2	2.45	0.51
2:B:68:LEU:HG	2:B:72:ARG:NH2	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:72:SER:HB2	4:D:74:HIS:CE1	2.46	0.51
5:E:17:SER:HB3	5:E:79:GLN:HB3	1.93	0.51
2:B:170:VAL:HB	2:B:189:ARG:HG2	1.93	0.50
2:B:95:VAL:HG22	2:B:122:PHE:HA	1.95	0.49
2:B:145:THR:CG2	2:B:158:LEU:H	2.26	0.49
4:D:25:TYR:CD2	4:D:33:LEU:HD11	2.48	0.49
2:B:67:ILE:O	2:B:71:LYS:HG2	2.12	0.49
1:A:108:VAL:HG21	1:A:118:ILE:HD11	1.95	0.48
2:B:37:ILE:HG13	2:B:38:VAL:N	2.29	0.48
4:D:33:LEU:HD13	4:D:73:PHE:HB2	1.95	0.48
5:E:29:ALA:O	5:E:68:ARG:NH2	2.35	0.48
1:A:71:ILE:HD13	3:C:12:GLY:HA2	1.96	0.48
2:B:10:GLN:HB2	2:B:31:ILE:HB	1.95	0.48
1:A:26:PHE:CE1	2:B:86:GLU:HG2	2.49	0.47
1:A:104:LEU:HD23	1:A:104:LEU:HA	1.79	0.47
2:B:69:GLU:HB3	4:D:51:THR:HG21	1.95	0.47
2:B:37:ILE:HA	2:B:51:THR:HB	1.96	0.47
2:B:132:PHE:HB2	2:B:172:THR:HB	1.97	0.47
1:A:74:LYS:HE3	1:A:74:LYS:HB2	1.81	0.47
2:B:37:ILE:HG13	2:B:38:VAL:H	1.79	0.46
2:B:38:VAL:HG13	2:B:58:ALA:HB2	1.97	0.46
4:D:34:PHE:CE2	4:D:93:PRO:HD3	2.51	0.46
5:E:131:PRO:HD2	5:E:202:TRP:CZ2	2.50	0.46
5:E:193:SER:C	5:E:194:ARG:HD3	2.40	0.46
5:E:143:THR:OG1	5:E:196:ARG:HD2	2.16	0.45
1:A:158:GLU:HG2	1:A:160:TYR:CE1	2.52	0.45
4:D:126:ASP:HA	5:E:129:PHE:HD1	1.81	0.45
5:E:180:GLU:HG3	5:E:188:ARG:HB2	1.98	0.44
4:D:97:SER:CB	5:E:54:VAL:HG11	2.47	0.44
1:A:39:LYS:HE3	1:A:56:GLN:HG2	2.00	0.44
2:B:97:PRO:HB3	2:B:122:PHE:HB3	1.99	0.43
4:D:134:VAL:HG22	4:D:177:TRP:HB3	1.99	0.43
5:E:173:THR:HG22	5:E:193:SER:OG	2.19	0.43
1:A:56:GLN:O	1:A:60:THR:HG23	2.19	0.42
2:B:75:VAL:O	2:B:79:CYS:HB2	2.20	0.42
2:B:89:THR:OG1	2:B:90:THR:N	2.53	0.42
5:E:124:PRO:HB3	5:E:151:PHE:HB3	2.01	0.42
4:D:193:ILE:O	4:D:194:ILE:HG13	2.19	0.42
5:E:59:LEU:O	5:E:61:LYS:HD2	2.20	0.42
5:E:181:GLN:CB	5:E:184:LEU:HD13	2.50	0.42
2:B:87:LEU:HA	2:B:91:LEU:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:137:PHE:O	4:D:173:SER:HA	2.20	0.41
5:E:21:TRP:CH2	5:E:23:ASN:HB2	2.56	0.41
1:A:7:SER:HB3	1:A:10:VAL:HG23	2.02	0.41
1:A:11:ASN:HB2	2:B:11:PHE:HB3	2.02	0.41
2:B:133:ARG:HB2	2:B:138:GLU:HB2	2.02	0.41
5:E:123:PRO:HD3	5:E:231:PRO:HB3	2.02	0.41
2:B:68:LEU:HD13	2:B:68:LEU:HA	1.92	0.41
1:A:81:ALA:HB1	1:A:112:PHE:CE1	2.54	0.41
4:D:126:ASP:OD1	4:D:127:SER:N	2.54	0.40
2:B:81:HIS:CD2	3:C:3:PHE:HD2	2.39	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	180/254 (71%)	168 (93%)	12 (7%)	0	100	100
2	B	174/261 (67%)	158 (91%)	16 (9%)	0	100	100
3	C	10/12 (83%)	10 (100%)	0	0	100	100
4	D	187/206 (91%)	174 (93%)	13 (7%)	0	100	100
5	E	241/245 (98%)	225 (93%)	16 (7%)	0	100	100
All	All	792/978 (81%)	735 (93%)	57 (7%)	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	166/223 (74%)	163 (98%)	3 (2%)	51	80
2	B	162/229 (71%)	157 (97%)	5 (3%)	35	69
3	C	10/10 (100%)	10 (100%)	0	100	100
4	D	164/182 (90%)	158 (96%)	6 (4%)	30	63
5	E	204/208 (98%)	198 (97%)	6 (3%)	37	71
All	All	706/852 (83%)	686 (97%)	20 (3%)	38	71

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	VAL
1	A	116	VAL
1	A	164	VAL
2	B	68	LEU
2	B	95	VAL
2	B	116	VAL
2	B	129	VAL
2	B	142	VAL
4	D	48	LEU
4	D	80	VAL
4	D	146	VAL
4	D	162	LEU
4	D	164	MET
4	D	194	ILE
5	E	40	GLN
5	E	58	GLN
5	E	72	VAL
5	E	83	LEU
5	E	200	THR
5	E	236	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
1	A	110	ASN
2	B	150	ASN

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Mol	Chain	Res	Type
2	B	156	GLN
4	D	2	ASN
5	E	16	GLN
5	E	28	HIS
5	E	79	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](#)

5 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	NAG	B	301	2	14,14,15	0.63	0	17,19,21	0.61	0
7	GOL	A	303	-	5,5,5	0.35	0	5,5,5	0.25	0
6	NAG	A	301	1	14,14,15	2.19	2 (14%)	17,19,21	2.24	3 (17%)
7	GOL	E	301	-	5,5,5	0.34	0	5,5,5	0.29	0
6	NAG	A	302	1	14,14,15	0.34	0	17,19,21	0.54	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	NAG	B	301	2	-	4/6/23/26	0/1/1/1
7	GOL	A	303	-	-	0/4/4/4	-
6	NAG	A	301	1	-	2/6/23/26	0/1/1/1
7	GOL	E	301	-	-	4/4/4/4	-
6	NAG	A	302	1	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	301	NAG	O5-C1	7.18	1.55	1.43
6	A	301	NAG	C1-C2	3.50	1.57	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	301	NAG	C1-O5-C5	7.70	122.51	112.19
6	A	301	NAG	C1-C2-N2	2.93	115.05	110.43
6	A	301	NAG	C2-N2-C7	2.33	126.02	122.90

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	301	NAG	C1-C2-N2-C7
6	A	302	NAG	O5-C5-C6-O6
6	A	302	NAG	C4-C5-C6-O6
6	B	301	NAG	C8-C7-N2-C2
6	B	301	NAG	O7-C7-N2-C2
6	B	301	NAG	C4-C5-C6-O6
6	B	301	NAG	O5-C5-C6-O6
7	E	301	GOL	O1-C1-C2-C3
7	E	301	GOL	C1-C2-C3-O3
7	E	301	GOL	O1-C1-C2-O2
7	E	301	GOL	O2-C2-C3-O3
6	A	301	NAG	O5-C5-C6-O6

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	182/254 (71%)	-0.04	2 (1%) 78 70	29, 51, 76, 95	0
2	B	178/261 (68%)	0.25	7 (3%) 43 34	28, 61, 105, 122	0
3	C	12/12 (100%)	-0.05	1 (8%) 17 12	35, 46, 69, 76	0
4	D	191/206 (92%)	0.69	19 (9%) 13 9	40, 72, 118, 131	0
5	E	243/245 (99%)	0.40	11 (4%) 38 30	31, 69, 104, 120	0
All	All	806/978 (82%)	0.33	40 (4%) 34 26	28, 62, 106, 131	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	178	SER	3.9
1	A	181	ILE	3.9
2	B	160	MET	3.8
2	B	168	GLY	3.8
4	D	53	ALA	3.7
2	B	114	LEU	3.6
5	E	244	ALA	3.6
4	D	176	ALA	3.4
4	D	115	GLN	3.4
4	D	193	ILE	3.3
4	D	183	PHE	3.3
4	D	141	ASP	3.1
4	D	28	THR	3.0
4	D	116	ASN	2.9
2	B	164	THR	2.7
4	D	152	SER	2.7
4	D	78	GLY	2.7
2	B	165	PRO	2.7
5	E	49	GLN	2.7
4	D	129	SER	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	166	GLN	2.6
5	E	184	LEU	2.6
4	D	182	ASP	2.6
4	D	145	ASN	2.5
4	D	150	LYS	2.5
3	C	12	GLY	2.5
5	E	122	PHE	2.5
4	D	132	LYS	2.3
4	D	194	ILE	2.3
5	E	23	ASN	2.3
5	E	38	LEU	2.2
5	E	120	ASN	2.2
5	E	73	ASP	2.1
4	D	3	SER	2.1
4	D	184	ALA	2.1
5	E	228	ARG	2.1
1	A	78	SER	2.1
5	E	152	TYR	2.0
2	B	162	GLU	2.0
5	E	54	VAL	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
6	NAG	B	301	14/15	0.33	0.19	94,116,123,124	0
6	NAG	A	301	14/15	0.51	0.21	87,105,115,123	0
7	GOL	E	301	6/6	0.73	0.26	65,72,78,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	GOL	A	303	6/6	0.84	0.23	59,73,77,77	0
6	NAG	A	302	14/15	0.88	0.11	51,89,96,98	0

6.5 Other polymers [i](#)

There are no such residues in this entry.