



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 19, 2022 – 08:06 AM EST

PDB ID : 6XCO  
Title : Immune receptor complex  
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Deposited on : 2020-06-08  
Resolution : 2.90 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](mailto: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.

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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 : 2.25  
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) : 2.25

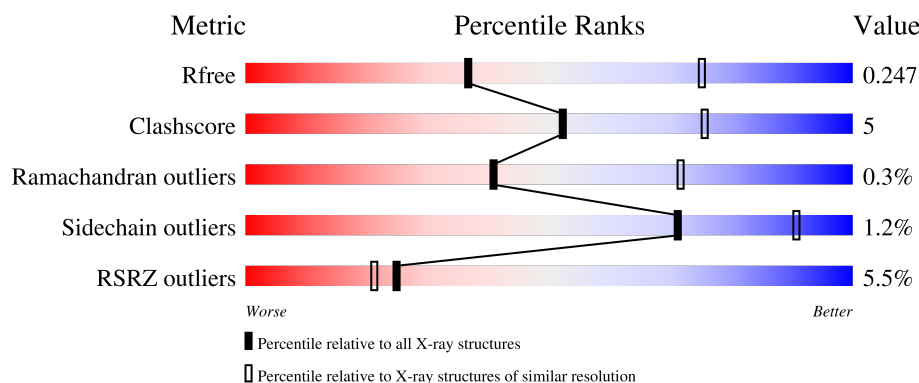
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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  $\geq 3$ , 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	193	
2	B	230	
3	D	205	
4	E	240	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	A	202	-	-	-	X
6	GOL	D	302	-	-	-	X
6	GOL	E	302	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6447 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 MHC class II HLA-DQ-alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	182	Total	C	N	O	S	0	0	0
			1451	934	238	276	3			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	72	CYS	ILE	engineered mutation	UNP Q30069
A	182	SER	-	expression tag	UNP Q30069
A	183	THR	-	expression tag	UNP Q30069
A	184	GLY	-	expression tag	UNP Q30069
A	185	GLY	-	expression tag	UNP Q30069
A	186	ASP	-	expression tag	UNP Q30069
A	187	ASP	-	expression tag	UNP Q30069
A	188	ASP	-	expression tag	UNP Q30069
A	189	ASP	-	expression tag	UNP Q30069
A	190	LYS	-	expression tag	UNP Q30069

- Molecule 2 is a protein called Hybrid Insulin Peptide, MHC class II HLA-DQ-beta-1 fusion.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	195	Total	C	N	O	S	0	0	0
			1561	988	272	294	7			

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	28	GLY	-	linker	PDB ?
B	29	SER	-	linker	PDB ?
B	30	GLY	-	linker	PDB ?
B	31	GLY	-	linker	PDB ?
B	32	SER	-	linker	PDB ?
B	33	ILE	-	linker	PDB ?

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Chain	Residue	Modelled	Actual	Comment	Reference
B	34	GLU	-	linker	PDB ?
B	35	GLY	-	linker	PDB ?
B	36	ARG	-	linker	PDB ?
B	37	GLY	-	linker	PDB ?
B	38	GLY	-	linker	PDB ?
B	39	SER	-	linker	PDB ?
B	40	GLY	-	linker	PDB ?
B	41	ALA	-	linker	PDB ?
B	42	SER	-	linker	PDB ?
B	235	THR	-	expression tag	UNP O19707
B	236	GLY	-	expression tag	UNP O19707
B	237	GLY	-	expression tag	UNP O19707
B	238	ASP	-	expression tag	UNP O19707
B	239	ASP	-	expression tag	UNP O19707
B	240	ASP	-	expression tag	UNP O19707
B	241	ASP	-	expression tag	UNP O19707
B	242	LYS	-	expression tag	UNP O19707

- Molecule 3 is a protein called T-CELL-RECEPTOR, A1.9-alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	187	Total	C	N	O	S	0	0	0
			1416	884	236	290	6			

- Molecule 4 is a protein called T-CELL-RECEPTOR, A1.9-beta chain.

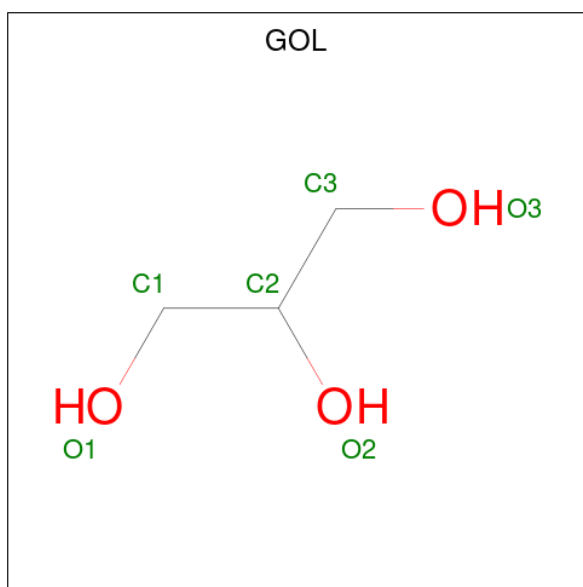
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	238	Total	C	N	O	S	0	0	0
			1869	1175	333	355	6			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



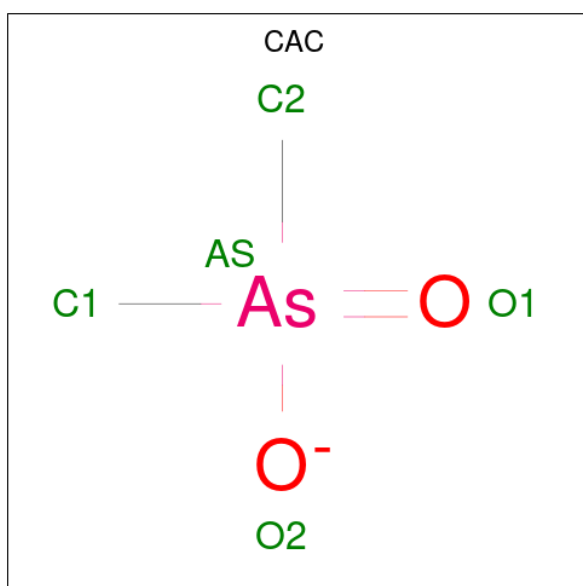
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		
6	D	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 CACODYLATE ION (three-letter code: CAC) (formula:  $C_2H_6AsO_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	As	C	O	0	0
			5	1	2	2		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	17	Total	O	0	0
			17	17		
8	B	10	Total	O	0	0
			10	10		
8	D	17	Total	O	0	0
			17	17		

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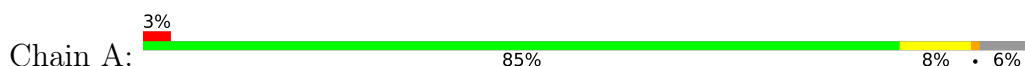
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	E	23	Total	O	0	0
			23	23		



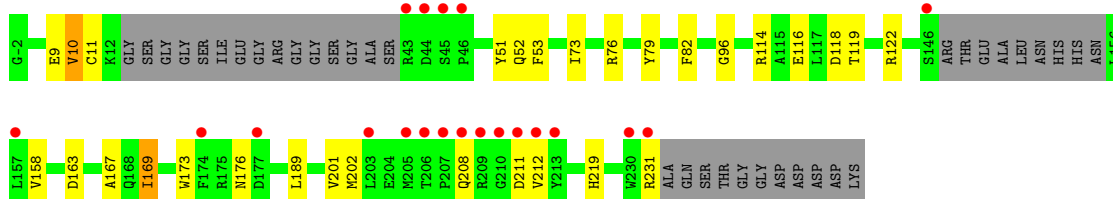
### 3 Residue-property plots [i](#)

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.

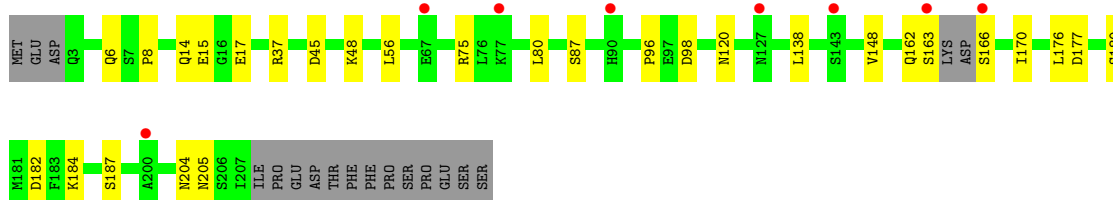
- Molecule 1: MHC class II HLA-DQ-alpha chain



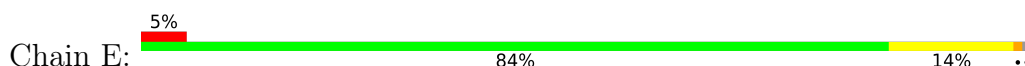
- Molecule 2: Hybrid Insulin Peptide, MHC class II HLA-DQ-beta-1 fusion

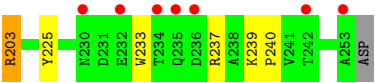


- Molecule 3: T-CELL-RECEPTOR, A1.9-alpha chain



- Molecule 4: T-CELL-RECEPTOR, A1.9-beta chain





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.29Å 104.31Å 69.32Å 90.00° 114.91° 90.00°	Depositor
Resolution (Å)	40.14 – 2.90 40.14 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (40.14-2.90) 100.0 (40.14-2.90)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.06 (at 2.90Å)	Xtriage
Refinement program	PHENIX 1.15_3459	Depositor
R, $R_{free}$	0.207 , 0.247 0.206 , 0.247	Depositor DCC
$R_{free}$ test set	967 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.8	Xtriage
Anisotropy	0.568	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 37.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.038 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6447	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.96% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: NAG, GOL, CAC

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	0.25	0/1494	0.43	0/2042
2	B	0.32	0/1597	0.45	0/2178
3	D	0.25	0/1443	0.44	0/1958
4	E	0.34	1/1919 (0.1%)	0.44	1/2612 (0.0%)
All	All	0.30	1/6453 (0.0%)	0.44	1/8790 (0.0%)

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
4	E	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	58	SER	C-N	9.76	1.56	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	58	SER	C-N-CA	5.46	135.35	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	E	58	SER	Mainchain

## 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	1451	0	1371	12	0
2	B	1561	0	1487	24	0
3	D	1416	0	1324	17	0
4	E	1869	0	1752	23	0
5	A	28	0	26	1	0
5	B	14	0	13	0	0
6	A	6	0	8	0	0
6	B	6	0	8	0	0
6	D	12	0	16	0	0
6	E	12	0	16	1	0
7	A	5	0	0	0	0
8	A	17	0	0	0	0
8	B	10	0	0	0	0
8	D	17	0	0	0	0
8	E	23	0	0	0	0
All	All	6447	0	6021	68	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 5.

All (68) 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)
1:A:11:ASN:HB2	2:B:53:PHE:HB3	1.75	0.69
1:A:76:ARG:NH1	2:B:9:GLU:OE1	2.25	0.68
1:A:12:LEU:HD11	1:A:115:PRO:HG3	1.77	0.66
2:B:10:VAL:HG12	2:B:11:CYS:N	2.10	0.65
4:E:21:LEU:HD22	4:E:119:THR:HG21	1.79	0.65
3:D:8:PRO:O	3:D:120:ASN:ND2	2.30	0.64
2:B:52:GLN:HB2	2:B:73:ILE:HB	1.82	0.61
1:A:70:LEU:HD13	2:B:51:TYR:HB2	1.84	0.60
4:E:63:GLU:HA	4:E:80:GLN:HB3	1.84	0.59
1:A:66:LEU:HD13	2:B:51:TYR:HD2	1.69	0.58
2:B:10:VAL:CG1	2:B:11:CYS:N	2.67	0.57
3:D:163:SER:HG	3:D:166:SER:N	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:37:ARG:HH22	4:E:110:ARG:HD3	1.70	0.56
3:D:56:LEU:HD13	3:D:80:LEU:HB2	1.87	0.55
2:B:176:ASN:HD21	2:B:211:ASP:HA	1.71	0.55
2:B:118:ASP:OD1	2:B:122:ARG:HD2	2.07	0.54
4:E:233:TRP:HB2	4:E:239:LYS:HE2	1.89	0.54
3:D:187:SER:HB2	4:E:203:ARG:HD3	1.89	0.54
4:E:19:VAL:HG13	4:E:94:LEU:HD11	1.89	0.53
1:A:97:VAL:HG22	1:A:103:ASN:HD22	1.73	0.52
4:E:132:PRO:HD3	4:E:240:PRO:HB3	1.90	0.52
4:E:57:PHE:CZ	4:E:109:GLU:HG3	2.44	0.52
2:B:116:GLU:HA	2:B:119:THR:HB	1.91	0.52
4:E:183:ASP:OD2	4:E:201:SER:HB3	2.10	0.51
3:D:75:ARG:NH2	3:D:98:ASP:OD2	2.44	0.50
3:D:15:GLU:OE2	3:D:96:PRO:HD3	2.11	0.50
4:E:40:SER:HB2	4:E:105:ALA:HB3	1.92	0.50
4:E:139:GLU:OE2	6:E:302:GOL:H2	2.12	0.50
4:E:164:HIS:HB3	4:E:225:TYR:HB2	1.93	0.50
2:B:158:VAL:HG22	2:B:202:MET:HG2	1.94	0.49
2:B:176:ASN:ND2	2:B:211:ASP:OD2	2.45	0.49
2:B:176:ASN:OD1	2:B:212:VAL:N	2.45	0.49
2:B:51:TYR:HH	2:B:79:TYR:HH	1.61	0.48
4:E:57:PHE:CE1	4:E:109:GLU:CG	2.97	0.47
2:B:169:ILE:HD12	2:B:219:HIS:HD2	1.80	0.47
3:D:37:ARG:NH2	4:E:110:ARG:HD3	2.29	0.47
1:A:176:LYS:HD3	1:A:176:LYS:HA	1.83	0.46
2:B:79:TYR:HD1	2:B:96:GLY:HA3	1.81	0.45
2:B:118:ASP:OD1	2:B:122:ARG:NH1	2.48	0.45
3:D:176:LEU:HD13	3:D:184:LYS:HD2	1.98	0.45
4:E:56:TYR:OH	4:E:78:GLY:C	2.54	0.45
4:E:43:GLN:HB2	4:E:53:LEU:HD21	1.98	0.45
4:E:56:TYR:CE1	4:E:79:ARG:HA	2.52	0.45
4:E:57:PHE:CE1	4:E:109:GLU:HG3	2.53	0.44
2:B:82:PHE:HZ	2:B:114:ARG:HG2	1.83	0.44
1:A:97:VAL:HG21	1:A:178:TRP:CZ2	2.53	0.44
4:E:39:VAL:HG11	4:E:87:SER:HB3	1.99	0.44
2:B:167:ALA:HB1	2:B:189:LEU:HD21	1.99	0.44
4:E:182:THR:HG23	4:E:202:SER:HB2	2.00	0.44
1:A:160:ILE:HD12	1:A:177:HIS:HE1	1.82	0.43
3:D:177:ASP:HB3	3:D:180:SER:HB2	1.99	0.43
1:A:142:ASP:HB2	2:B:76:ARG:HH21	1.82	0.43
3:D:162:GLN:HG2	3:D:163:SER:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:202:NAG:H3	5:A:202:NAG:H83	1.99	0.43
4:E:130:VAL:O	4:E:237:ARG:NH1	2.50	0.43
3:D:138:LEU:HB2	3:D:148:VAL:HG23	2.01	0.42
3:D:204:ASN:HB3	3:D:205:ASN:H	1.53	0.42
3:D:80:LEU:HD12	3:D:87:SER:HB2	2.00	0.42
4:E:55:GLU:OE1	4:E:66:ARG:HB3	2.20	0.42
4:E:13:LYS:HG3	4:E:19:VAL:HG12	2.02	0.41
3:D:45:ASP:HB2	3:D:48:LYS:HB2	2.03	0.41
2:B:208:GLN:N	2:B:211:ASP:OD1	2.46	0.41
3:D:14:GLN:HG2	3:D:17:GLU:OE1	2.21	0.41
3:D:162:GLN:HA	3:D:170:ILE:HB	2.03	0.41
2:B:173:TRP:HE1	2:B:201:VAL:HG23	1.86	0.40
1:A:88:GLU:HB3	1:A:110:ASP:HB3	2.02	0.40
1:A:94:LYS:HE3	2:B:163:ASP:OD2	2.22	0.40
2:B:118:ASP:HA	2:B:122:ARG:HB2	2.04	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	180/193 (93%)	175 (97%)	4 (2%)	1 (1%)	25	58
2	B	189/230 (82%)	176 (93%)	13 (7%)	0	100	100
3	D	183/205 (89%)	173 (94%)	10 (6%)	0	100	100
4	E	236/240 (98%)	225 (95%)	10 (4%)	1 (0%)	34	66
All	All	788/868 (91%)	749 (95%)	37 (5%)	2 (0%)	41	71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	PRO
4	E	109	GLU

### 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	162/176 (92%)	161 (99%)	1 (1%)	86	96
2	B	169/200 (84%)	166 (98%)	3 (2%)	59	85
3	D	155/181 (86%)	153 (99%)	2 (1%)	69	90
4	E	200/210 (95%)	198 (99%)	2 (1%)	76	92
All	All	686/767 (89%)	678 (99%)	8 (1%)	71	91

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	LEU
2	B	10	VAL
2	B	169	ILE
2	B	231	ARG
3	D	6	GLN
3	D	182	ASP
4	E	54	PHE
4	E	203	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

10 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	301	-	5,5,5	0.92	0	5,5,5	0.97	0
5	NAG	A	202	1	14,14,15	0.60	0	17,19,21	1.56	4 (23%)
7	CAC	A	204	-	0,4,4	-	-	0,6,6	-	-
6	GOL	B	302	-	5,5,5	0.92	0	5,5,5	0.99	0
6	GOL	D	301	-	5,5,5	0.90	0	5,5,5	1.01	0
6	GOL	E	302	-	5,5,5	0.93	0	5,5,5	0.99	0
6	GOL	A	203	-	5,5,5	0.89	0	5,5,5	1.02	0
6	GOL	D	302	-	5,5,5	0.94	0	5,5,5	0.97	0
5	NAG	B	301	2	14,14,15	1.24	1 (7%)	17,19,21	1.70	4 (23%)
5	NAG	A	201	1	14,14,15	0.69	1 (7%)	17,19,21	0.80	1 (5%)

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	301	-	-	1/4/4/4	-
5	NAG	A	202	1	-	4/6/23/26	0/1/1/1
6	GOL	B	302	-	-	0/4/4/4	-
6	GOL	D	301	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	E	302	-	-	0/4/4/4	-
6	GOL	A	203	-	-	0/4/4/4	-
6	GOL	D	302	-	-	2/4/4/4	-
5	NAG	B	301	2	-	5/6/23/26	0/1/1/1
5	NAG	A	201	1	-	4/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	301	NAG	O5-C1	-4.43	1.36	1.43
5	A	201	NAG	O5-C1	2.24	1.47	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	301	NAG	C2-N2-C7	4.40	129.18	122.90
5	A	202	NAG	C2-N2-C7	4.40	129.16	122.90
5	B	301	NAG	C3-C4-C5	3.63	116.71	110.24
5	A	201	NAG	C1-O5-C5	2.81	116.00	112.19
5	B	301	NAG	C4-C3-C2	2.62	114.86	111.02
5	A	202	NAG	C1-O5-C5	2.61	115.73	112.19
5	B	301	NAG	C1-C2-N2	2.34	114.49	110.49
5	A	202	NAG	C3-C4-C5	2.33	114.39	110.24
5	A	202	NAG	C1-C2-N2	2.06	114.02	110.49

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	301	NAG	C4-C5-C6-O6
5	A	201	NAG	O5-C5-C6-O6
5	A	201	NAG	C4-C5-C6-O6
5	B	301	NAG	O5-C5-C6-O6
5	A	201	NAG	C8-C7-N2-C2
5	A	201	NAG	O7-C7-N2-C2
5	A	202	NAG	C8-C7-N2-C2
5	A	202	NAG	O7-C7-N2-C2
5	B	301	NAG	C8-C7-N2-C2
5	B	301	NAG	O7-C7-N2-C2
5	A	202	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	B	301	NAG	C3-C2-N2-C7
6	D	302	GOL	C1-C2-C3-O3
6	D	302	GOL	O2-C2-C3-O3
5	A	202	NAG	C3-C2-N2-C7
6	E	301	GOL	C1-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	202	NAG	1	0
6	E	302	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	182/193 (94%)	0.32	5 (2%) 54 50	37, 50, 77, 102	0
2	B	195/230 (84%)	0.64	20 (10%) 6 5	35, 52, 87, 104	0
3	D	187/205 (91%)	0.46	8 (4%) 35 31	39, 58, 89, 113	0
4	E	238/240 (99%)	0.43	11 (4%) 32 29	38, 51, 77, 98	0
All	All	802/868 (92%)	0.46	44 (5%) 25 21	35, 52, 83, 113	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	43	ARG	4.8
4	E	192	ALA	4.8
4	E	253	ALA	4.7
2	B	209	ARG	4.6
2	B	213	TYR	4.6
2	B	206	THR	4.3
3	D	143	SER	4.1
4	E	194	ASN	4.1
2	B	208	GLN	4.1
2	B	212	VAL	4.1
2	B	146	SER	4.1
2	B	207	PRO	4.0
2	B	211	ASP	3.7
3	D	163	SER	3.5
2	B	205	MET	3.5
2	B	157	LEU	3.4
2	B	44	ASP	3.4
2	B	177	ASP	3.2
1	A	177	HIS	3.1
2	B	45	SER	3.0
2	B	230	TRP	2.9

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Mol	Chain	Res	Type	RSRZ
4	E	235	GLN	2.8
2	B	174	PHE	2.7
1	A	180	PRO	2.7
4	E	234	THR	2.7
2	B	210	GLY	2.7
4	E	232	GLU	2.6
3	D	127	ASN	2.5
2	B	46	PRO	2.5
2	B	231	ARG	2.4
1	A	179	GLU	2.4
4	E	127	LEU	2.3
1	A	166	GLU	2.3
4	E	230	ASN	2.3
1	A	162	ASP	2.2
3	D	90	HIS	2.2
2	B	203	LEU	2.2
4	E	236	ASP	2.1
3	D	67	GLU	2.1
4	E	16	GLY	2.1
3	D	200	ALA	2.0
3	D	166	SER	2.0
4	E	242	THR	2.0
3	D	77	LYS	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 monosaccharides 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, 95<sup>th</sup> 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	GOL	E	302	6/6	0.46	0.42	78,81,87,89	0
5	NAG	A	202	14/15	0.63	0.46	118,128,131,133	0
6	GOL	B	302	6/6	0.67	0.37	73,86,87,94	0
5	NAG	B	301	14/15	0.67	0.29	101,112,118,119	0
6	GOL	E	301	6/6	0.72	0.32	76,81,86,87	0
6	GOL	D	302	6/6	0.74	0.42	67,81,84,89	0
5	NAG	A	201	14/15	0.76	0.38	104,111,117,121	0
6	GOL	D	301	6/6	0.80	0.26	80,82,85,85	0
7	CAC	A	204	5/5	0.82	0.24	147,148,149,149	0
6	GOL	A	203	6/6	0.87	0.32	72,75,76,77	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.