



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 06:27 pm GMT

PDB ID : 3S5L  
Title : Crystal structure of CD4 mutant bound to HLA-DR1  
Authors : Li, Y.  
Deposited on : 2011-05-23  
Resolution : 2.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

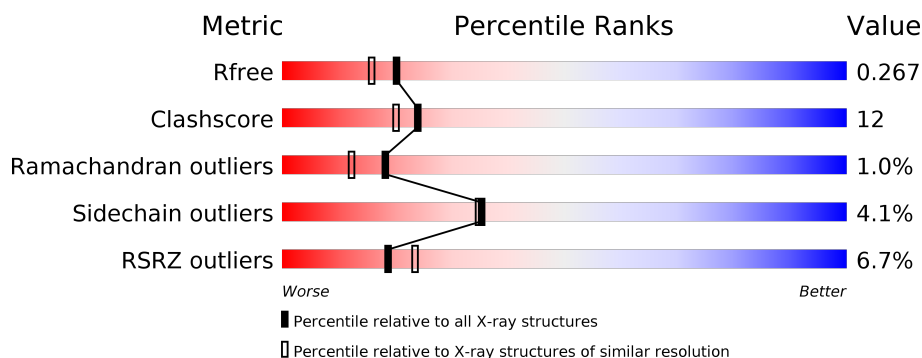
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
$R_{free}$	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	182	
1	D	182	
2	B	193	
2	E	193	
3	C	13	
3	F	13	

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Mol	Chain	Length	Quality of chain
4	G	191	
4	H	191	

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	GOL	A	968	-	-	-	X
5	GOL	B	966	-	-	-	X
5	GOL	B	969	-	-	-	X
5	GOL	D	961	-	-	-	X
5	GOL	E	960	-	-	-	X
5	GOL	E	962	-	-	-	X
5	GOL	E	963	-	-	-	X
5	GOL	G	967	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9272 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, DR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	178	Total	C	N	O	S	0	0	0
			1464	949	237	273	5			
1	D	179	Total	C	N	O	S	0	0	0
			1467	950	238	274	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	177	GLN	HIS	CONFLICT	UNP P01903
D	177	GLN	HIS	CONFLICT	UNP P01903

- Molecule 2 is a protein called HLA class II histocompatibility antigen, DRB1-1 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	191	Total	C	N	O	S	0	0	0
			1533	961	275	290	7			
2	E	191	Total	C	N	O	S	0	0	0
			1545	971	276	291	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	EXPRESSION TAG	UNP P04229
E	0	MET	-	EXPRESSION TAG	UNP P04229

- Molecule 3 is a protein called HA peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	13	Total	C	N	O	0	0	0
			106	69	18	19			
3	F	13	Total	C	N	O	0	0	0
			106	69	18	19			

- Molecule 4 is a protein called T-cell surface glycoprotein CD4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	175	Total	C	N	O	S	0	0	0
			1369	860	244	261	4			
4	H	177	Total	C	N	O	S	0	0	0
			1354	851	241	258	4			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	-3	ASP	-	EXPRESSION TAG	UNP P01730
G	-2	LEU	-	EXPRESSION TAG	UNP P01730
G	-1	GLY	-	EXPRESSION TAG	UNP P01730
G	0	SER	-	EXPRESSION TAG	UNP P01730
G	40	TYR	GLN	ENGINEERED MUTATION	UNP P01730
G	45	TRP	THR	ENGINEERED MUTATION	UNP P01730
G	60	ARG	SER	ENGINEERED MUTATION	UNP P01730
G	63	ARG	ASP	ENGINEERED MUTATION	UNP P01730
G	179	ALA	-	EXPRESSION TAG	UNP P01730
G	180	ALA	-	EXPRESSION TAG	UNP P01730
G	181	ALA	-	EXPRESSION TAG	UNP P01730
G	182	HIS	-	EXPRESSION TAG	UNP P01730
G	183	HIS	-	EXPRESSION TAG	UNP P01730
G	184	HIS	-	EXPRESSION TAG	UNP P01730
G	185	HIS	-	EXPRESSION TAG	UNP P01730
G	186	HIS	-	EXPRESSION TAG	UNP P01730
G	187	HIS	-	EXPRESSION TAG	UNP P01730
H	-3	ASP	-	EXPRESSION TAG	UNP P01730
H	-2	LEU	-	EXPRESSION TAG	UNP P01730
H	-1	GLY	-	EXPRESSION TAG	UNP P01730
H	0	SER	-	EXPRESSION TAG	UNP P01730
H	40	TYR	GLN	ENGINEERED MUTATION	UNP P01730
H	45	TRP	THR	ENGINEERED MUTATION	UNP P01730
H	60	ARG	SER	ENGINEERED MUTATION	UNP P01730
H	63	ARG	ASP	ENGINEERED MUTATION	UNP P01730
H	179	ALA	-	EXPRESSION TAG	UNP P01730
H	180	ALA	-	EXPRESSION TAG	UNP P01730
H	181	ALA	-	EXPRESSION TAG	UNP P01730
H	182	HIS	-	EXPRESSION TAG	UNP P01730
H	183	HIS	-	EXPRESSION TAG	UNP P01730
H	184	HIS	-	EXPRESSION TAG	UNP P01730
H	185	HIS	-	EXPRESSION TAG	UNP P01730
H	186	HIS	-	EXPRESSION TAG	UNP P01730
H	187	HIS	-	EXPRESSION TAG	UNP P01730

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		
5	G	1	Total	C	O	0	0
			6	3	3		
5	G	1	Total	C	O	0	0
			6	3	3		
5	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	87	Total	O	0	0
			87	87		

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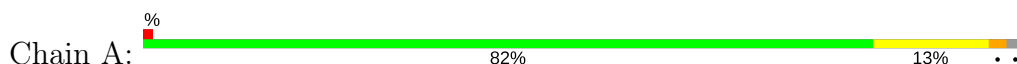
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	61	Total 61	O 61	0	0
6	B	57	Total 57	O 57	0	0
6	E	30	Total 30	O 30	0	0
6	C	5	Total 5	O 5	0	0
6	F	1	Total 1	O 1	0	0
6	G	16	Total 16	O 16	0	0
6	H	11	Total 11	O 11	0	0

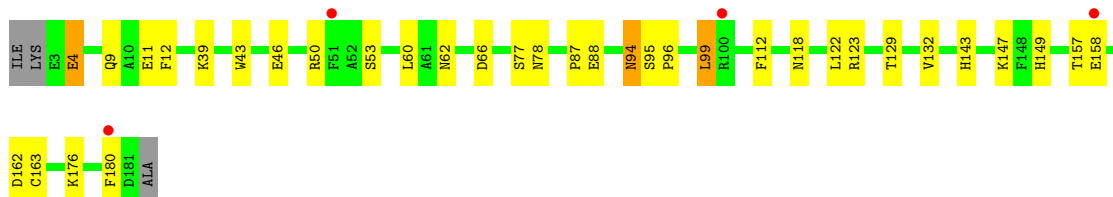
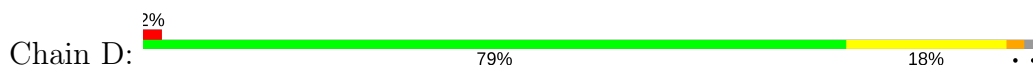
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

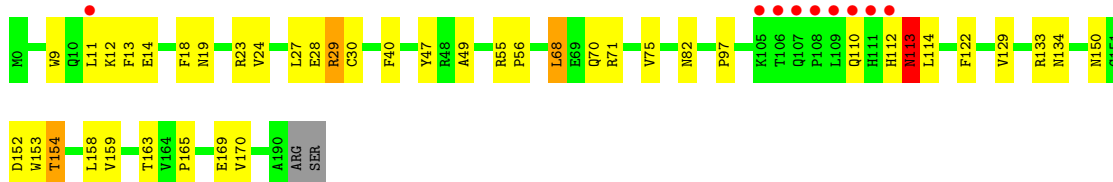
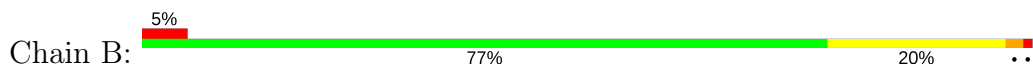
- Molecule 1: HLA class II histocompatibility antigen, DR alpha chain



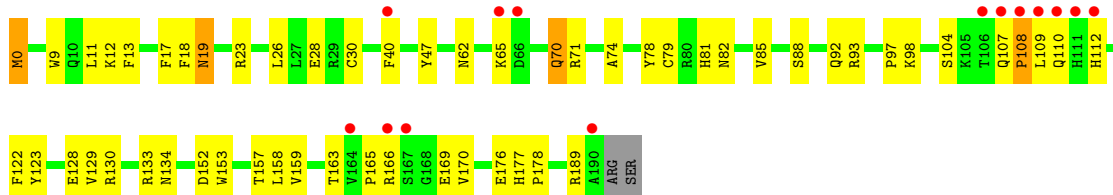
- Molecule 1: HLA class II histocompatibility antigen, DR alpha chain



- Molecule 2: HLA class II histocompatibility antigen, DRB1-1 beta chain



- Molecule 2: HLA class II histocompatibility antigen, DRB1-1 beta chain





- Chain H:
- 
- Sequence logo for Chain H. The y-axis represents frequency in bits (0.00 to 0.12). The x-axis shows positions 1 to 177. A color bar at the top indicates the distribution: 16% red, 61% green, 29% yellow, and 7% grey. A legend at the bottom identifies amino acids by color: ASP (grey), LEU (grey), GLY (grey), S0 (green), K1 (green), K2 (green), V3 (yellow), C16 (green), T17 (green), A18 (green), S19 (green), Q20 (green), H27 (green), V28 (green), K29 (yellow), N32 (yellow), Q33 (yellow), S49 (yellow), K50 (yellow), L51 (yellow), L52 (yellow), R58 (green), R59 (green), R60 (green), L61 (yellow), N66 (yellow), T60 (yellow), I70 (yellow), I83 (yellow), V86 (green), E87 (green), D88 (green), Q89 (green), V93 (yellow), T100 (yellow), T101 (yellow), A102 (yellow), K103 (yellow), S104 (red), D105 (green), T106 (green), H15 (grey), L159 (green), Q110 (green), G111 (green), Q112 (green), S113 (green), L114 (yellow), T115 (yellow).

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.20Å 119.70Å 137.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10 47.41 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-2.10) 99.8 (47.41-2.10)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.80 (at 2.10Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.234 , 0.268 0.233 , 0.267	Depositor DCC
$R_{free}$ test set	4566 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.4	Xtriage
Anisotropy	0.793	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 49.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9272	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.21 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.8222e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.56	0/1508	0.75	2/2056 (0.1%)
1	D	0.50	0/1511	0.73	1/2060 (0.0%)
2	B	0.52	0/1571	0.72	0/2130
2	E	0.46	0/1584	0.68	0/2150
3	C	0.49	0/107	0.82	0/141
3	F	0.39	0/107	0.83	0/141
4	G	0.38	0/1390	0.67	2/1873 (0.1%)
4	H	0.41	0/1374	0.68	0/1854
All	All	0.47	0/9152	0.71	5/12405 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	37	LEU	CA-CB-CG	5.87	128.81	115.30
4	G	41	GLY	N-CA-C	-5.64	98.99	113.10
1	D	163	CYS	N-CA-C	-5.42	96.37	111.00
1	A	88	GLU	N-CA-C	-5.22	96.90	111.00
1	A	163	CYS	N-CA-C	-5.03	97.43	111.00

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	1464	0	1404	24	0
1	D	1467	0	1403	27	0
2	B	1533	0	1442	36	0
2	E	1545	0	1466	43	0
3	C	106	0	119	12	0
3	F	106	0	119	5	0
4	G	1369	0	1385	50	0
4	H	1354	0	1339	54	0
5	A	6	0	8	0	0
5	B	12	0	16	0	0
5	D	6	0	8	0	0
5	E	18	0	24	1	0
5	G	12	0	16	3	0
5	H	6	0	8	3	0
6	A	87	0	0	1	0
6	B	57	0	0	0	0
6	C	5	0	0	0	0
6	D	61	0	0	0	0
6	E	30	0	0	1	0
6	F	1	0	0	0	0
6	G	16	0	0	0	0
6	H	11	0	0	0	0
All	All	9272	0	8757	222	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 12.

The worst 5 of 222 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:H:50:LYS:H	4:H:50:LYS:HD2	1.07	1.13
4:G:50:LYS:H	4:G:50:LYS:HE3	1.12	1.04
4:H:177:LEU:H	4:H:177:LEU:HD22	1.23	1.01
4:G:138:ILE:HG22	4:G:139:GLN:H	1.28	0.99
2:E:82:ASN:HD21	3:F:6:VAL:H	1.08	0.93

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	176/182 (97%)	172 (98%)	4 (2%)	0	100	100
1	D	177/182 (97%)	170 (96%)	6 (3%)	1 (1%)	28	24
2	B	189/193 (98%)	178 (94%)	9 (5%)	2 (1%)	17	11
2	E	189/193 (98%)	176 (93%)	12 (6%)	1 (0%)	32	28
3	C	11/13 (85%)	11 (100%)	0	0	100	100
3	F	11/13 (85%)	11 (100%)	0	0	100	100
4	G	171/191 (90%)	158 (92%)	10 (6%)	3 (2%)	10	4
4	H	173/191 (91%)	151 (87%)	18 (10%)	4 (2%)	7	3
All	All	1097/1158 (95%)	1027 (94%)	59 (5%)	11 (1%)	18	12

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	H	104	SER
4	G	148	GLN
4	H	113	SER
4	H	138	ILE
4	H	148	GLN

### 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	163/166 (98%)	159 (98%)	4 (2%)	53	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	163/166 (98%)	158 (97%)	5 (3%)	45	48
2	B	165/174 (95%)	159 (96%)	6 (4%)	40	41
2	E	168/174 (97%)	164 (98%)	4 (2%)	54	59
3	C	12/12 (100%)	10 (83%)	2 (17%)	2	1
3	F	12/12 (100%)	9 (75%)	3 (25%)	1	0
4	G	155/170 (91%)	146 (94%)	9 (6%)	23	20
4	H	146/170 (86%)	139 (95%)	7 (5%)	30	27
All	All	984/1044 (94%)	944 (96%)	40 (4%)	35	35

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	166	ARG
3	F	10	THR
4	H	152	GLN
3	C	10	THR
3	F	11	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	136	GLN
2	E	62	ASN
4	H	89	GLN
2	B	150	ASN
2	B	156	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry

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	$\# Z  > 2$
5	GOL	A	968	-	5,5,5	0.25	0	5,5,5	0.34	0
5	GOL	B	966	-	5,5,5	0.33	0	5,5,5	0.39	0
5	GOL	B	969	-	5,5,5	0.25	0	5,5,5	0.23	0
5	GOL	D	961	-	5,5,5	0.19	0	5,5,5	0.29	0
5	GOL	E	960	-	5,5,5	0.21	0	5,5,5	0.32	0
5	GOL	E	962	-	5,5,5	0.12	0	5,5,5	0.26	0
5	GOL	E	963	-	5,5,5	0.31	0	5,5,5	0.28	0
5	GOL	G	965	-	5,5,5	0.22	0	5,5,5	0.26	0
5	GOL	G	967	-	5,5,5	0.23	0	5,5,5	0.25	0
5	GOL	H	964	-	5,5,5	0.21	0	5,5,5	0.25	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
5	GOL	A	968	-	-	0/4/4/4	0/0/0/0
5	GOL	B	966	-	-	0/4/4/4	0/0/0/0
5	GOL	B	969	-	-	0/4/4/4	0/0/0/0
5	GOL	D	961	-	-	0/4/4/4	0/0/0/0
5	GOL	E	960	-	-	0/4/4/4	0/0/0/0
5	GOL	E	962	-	-	0/4/4/4	0/0/0/0
5	GOL	E	963	-	-	0/4/4/4	0/0/0/0
5	GOL	G	965	-	-	0/4/4/4	0/0/0/0
5	GOL	G	967	-	-	0/4/4/4	0/0/0/0
5	GOL	H	964	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	960	GOL	1	0
5	G	965	GOL	3	0
5	H	964	GOL	3	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	178/182 (97%)	0.07	1 (0%) 89 91	15, 25, 44, 61	0
1	D	179/182 (98%)	0.12	4 (2%) 62 67	16, 30, 57, 68	0
2	B	191/193 (98%)	0.02	9 (4%) 32 38	16, 29, 51, 95	0
2	E	191/193 (98%)	0.44	14 (7%) 16 20	19, 36, 63, 94	0
3	C	13/13 (100%)	0.07	0 100 100	26, 32, 39, 44	0
3	F	13/13 (100%)	0.47	1 (7%) 14 18	35, 43, 57, 58	0
4	G	175/191 (91%)	0.51	16 (9%) 10 13	25, 49, 74, 81	0
4	H	177/191 (92%)	0.60	30 (16%) 2 2	23, 45, 77, 85	0
All	All	1117/1158 (96%)	0.29	75 (6%) 19 23	15, 34, 72, 95	0

The worst 5 of 75 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	111	HIS	10.8
2	E	110	GLN	8.4
2	E	107	GLN	8.0
2	E	108	PRO	7.8
4	H	115	THR	5.0

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	GOL	B	969	6/6	0.77	0.22	7.84	63,64,64,64	0
5	GOL	B	966	6/6	0.85	0.20	6.81	34,37,41,46	0
5	GOL	D	961	6/6	0.87	0.19	4.17	51,56,57,59	0
5	GOL	G	967	6/6	0.91	0.24	3.81	55,56,58,58	0
5	GOL	E	960	6/6	0.83	0.18	3.80	61,62,62,63	0
5	GOL	A	968	6/6	0.87	0.15	2.77	34,41,44,48	0
5	GOL	E	963	6/6	0.86	0.19	2.60	37,41,43,44	0
5	GOL	E	962	6/6	0.91	0.19	2.40	50,51,51,52	0
5	GOL	H	964	6/6	0.86	0.23	-	55,55,56,60	0
5	GOL	G	965	6/6	0.81	0.23	-	54,54,56,56	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.