WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 03:44 PM GMT

PDB ID	:	4D8P
Title	:	Structural and functional studies of the trans-encoded HLA-DQ2.3 (DQA1*0 3:01/DQB1*02:01) molecule
Authors	:	Kim, C.-Y.; Hotta, K.; Mathews, I.I.; Chen, X.
Deposited on	:	2012-01-11
Resolution	:	3.05 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

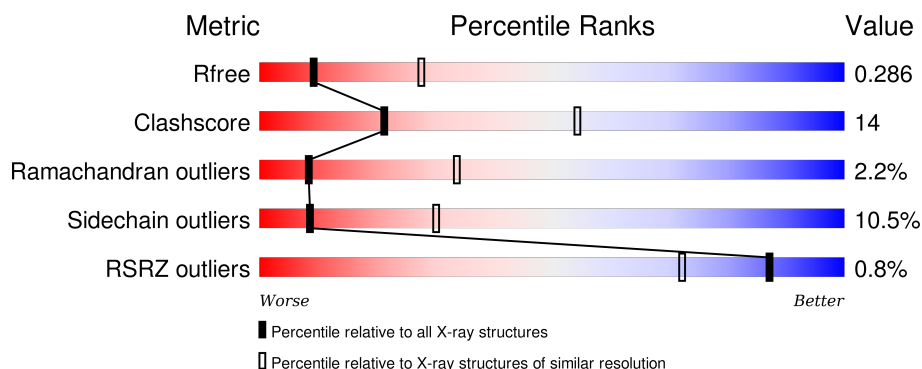|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1   Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 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	Percentile Ranks	Value
Rfree		0.286
Clashscore		14
Ramachandran outliers		2.2%
Sidechain outliers		10.5%
RSRZ outliers		0.8%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1191 (3.10-3.02)
Clashscore	102246	1303 (3.10-3.02)
Ramachandran outliers	100387	1254 (3.10-3.02)
Sidechain outliers	100360	1254 (3.10-3.02)
RSRZ outliers	91569	1197 (3.10-3.02)

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 >=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 <=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	213	57% 28% • 14%
1	C	213	60% 20% 6% 14%
2	B	250	% 48% 26% • 23%
2	D	250	% 45% 26% 6% 23%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6120 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-DQA1 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	184	Total	C	N	O	S	0	0	0
			1474	950	238	284	2			
1	C	183	Total	C	N	O	S	0	0	0
			1473	948	240	283	2			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	192	GLY	-	EXPRESSION TAG	UNP Q30063
A	193	GLY	-	EXPRESSION TAG	UNP Q30063
A	194	GLY	-	EXPRESSION TAG	UNP Q30063
A	195	SER	-	EXPRESSION TAG	UNP Q30063
A	196	GLY	-	EXPRESSION TAG	UNP Q30063
A	197	GLY	-	EXPRESSION TAG	UNP Q30063
A	198	GLY	-	EXPRESSION TAG	UNP Q30063
A	199	SER	-	EXPRESSION TAG	UNP Q30063
A	200	CYS	-	EXPRESSION TAG	UNP Q30063
A	201	SER	-	EXPRESSION TAG	UNP Q30063
A	202	ARG	-	EXPRESSION TAG	UNP Q30063
A	203	GLY	-	EXPRESSION TAG	UNP Q30063
A	204	GLY	-	EXPRESSION TAG	UNP Q30063
A	205	LEU	-	EXPRESSION TAG	UNP Q30063
A	206	GLU	-	EXPRESSION TAG	UNP Q30063
A	207	VAL	-	EXPRESSION TAG	UNP Q30063
A	208	LEU	-	EXPRESSION TAG	UNP Q30063
A	209	PHE	-	EXPRESSION TAG	UNP Q30063
A	210	GLN	-	EXPRESSION TAG	UNP Q30063
C	192	GLY	-	EXPRESSION TAG	UNP Q30063
C	193	GLY	-	EXPRESSION TAG	UNP Q30063
C	194	GLY	-	EXPRESSION TAG	UNP Q30063
C	195	SER	-	EXPRESSION TAG	UNP Q30063
C	196	GLY	-	EXPRESSION TAG	UNP Q30063
C	197	GLY	-	EXPRESSION TAG	UNP Q30063

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Chain	Residue	Modelled	Actual	Comment	Reference
C	198	GLY	-	EXPRESSION TAG	UNP Q30063
C	199	SER	-	EXPRESSION TAG	UNP Q30063
C	200	CYS	-	EXPRESSION TAG	UNP Q30063
C	201	SER	-	EXPRESSION TAG	UNP Q30063
C	202	ARG	-	EXPRESSION TAG	UNP Q30063
C	203	GLY	-	EXPRESSION TAG	UNP Q30063
C	204	GLY	-	EXPRESSION TAG	UNP Q30063
C	205	LEU	-	EXPRESSION TAG	UNP Q30063
C	206	GLU	-	EXPRESSION TAG	UNP Q30063
C	207	VAL	-	EXPRESSION TAG	UNP Q30063
C	208	LEU	-	EXPRESSION TAG	UNP Q30063
C	209	PHE	-	EXPRESSION TAG	UNP Q30063
C	210	GLN	-	EXPRESSION TAG	UNP Q30063

- Molecule 2 is a protein called Peptide from Gamma-gliadin, linker, MHC class II antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	193	Total	C	N	O	S	0	0	0
			1576	998	278	293	7			
2	D	193	Total	C	N	O	S	0	0	0
			1579	998	281	293	7			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-33	ARG	-	EXPRESSION TAG	UNP Q94G94
B	-32	ASP	-	EXPRESSION TAG	UNP Q94G94
B	-31	SER	-	EXPRESSION TAG	UNP Q94G94
B	-30	GLY	-	EXPRESSION TAG	UNP Q94G94
B	-26	GLU	GLN	ENGINEERED MUTATION	UNP Q94G94
B	-23	GLU	GLN	ENGINEERED MUTATION	UNP Q94G94
B	-14	GLY	-	LINKER	UNP Q94G94
B	-13	ALA	-	LINKER	UNP Q94G94
B	-12	GLY	-	LINKER	UNP Q94G94
B	-11	SER	-	LINKER	UNP Q94G94
B	-10	LEU	-	LINKER	UNP Q94G94
B	-9	VAL	-	LINKER	UNP Q94G94
B	-8	PRO	-	LINKER	UNP Q94G94
B	-7	ARG	-	LINKER	UNP Q94G94
B	-6	GLY	-	LINKER	UNP Q94G94
B	-5	SER	-	LINKER	UNP Q94G94
B	-4	GLY	-	LINKER	UNP Q94G94

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	LINKER	UNP Q94G94
B	-2	GLY	-	LINKER	UNP Q94G94
B	-1	GLY	-	LINKER	UNP Q94G94
B	0	SER	-	LINKER	UNP Q94G94
B	199	GLY	-	EXPRESSION TAG	UNP Q5Y7D3
B	200	GLY	-	EXPRESSION TAG	UNP Q5Y7D3
B	201	GLY	-	EXPRESSION TAG	UNP Q5Y7D3
B	202	SER	-	EXPRESSION TAG	UNP Q5Y7D3
B	203	GLY	-	EXPRESSION TAG	UNP Q5Y7D3
B	204	GLY	-	EXPRESSION TAG	UNP Q5Y7D3
B	205	GLY	-	EXPRESSION TAG	UNP Q5Y7D3
B	206	SER	-	EXPRESSION TAG	UNP Q5Y7D3
B	207	CYS	-	EXPRESSION TAG	UNP Q5Y7D3
B	208	SER	-	EXPRESSION TAG	UNP Q5Y7D3
B	209	ARG	-	EXPRESSION TAG	UNP Q5Y7D3
B	210	GLY	-	EXPRESSION TAG	UNP Q5Y7D3
B	211	GLY	-	EXPRESSION TAG	UNP Q5Y7D3
B	212	LEU	-	EXPRESSION TAG	UNP Q5Y7D3
B	213	GLU	-	EXPRESSION TAG	UNP Q5Y7D3
B	214	VAL	-	EXPRESSION TAG	UNP Q5Y7D3
B	215	LEU	-	EXPRESSION TAG	UNP Q5Y7D3
B	216	PHE	-	EXPRESSION TAG	UNP Q5Y7D3
B	217	GLN	-	EXPRESSION TAG	UNP Q5Y7D3
D	-33	ARG	-	EXPRESSION TAG	UNP Q94G94
D	-32	ASP	-	EXPRESSION TAG	UNP Q94G94
D	-31	SER	-	EXPRESSION TAG	UNP Q94G94
D	-30	GLY	-	EXPRESSION TAG	UNP Q94G94
D	-26	GLU	GLN	ENGINEERED MUTATION	UNP Q94G94
D	-23	GLU	GLN	ENGINEERED MUTATION	UNP Q94G94
D	-14	GLY	-	LINKER	UNP Q94G94
D	-13	ALA	-	LINKER	UNP Q94G94
D	-12	GLY	-	LINKER	UNP Q94G94
D	-11	SER	-	LINKER	UNP Q94G94
D	-10	LEU	-	LINKER	UNP Q94G94
D	-9	VAL	-	LINKER	UNP Q94G94
D	-8	PRO	-	LINKER	UNP Q94G94
D	-7	ARG	-	LINKER	UNP Q94G94
D	-6	GLY	-	LINKER	UNP Q94G94
D	-5	SER	-	LINKER	UNP Q94G94
D	-4	GLY	-	LINKER	UNP Q94G94
D	-3	GLY	-	LINKER	UNP Q94G94
D	-2	GLY	-	LINKER	UNP Q94G94

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	GLY	-	LINKER	UNP Q94G94
D	0	SER	-	LINKER	UNP Q94G94
D	199	GLY	-	EXPRESSION TAG	UNP Q5Y7D3
D	200	GLY	-	EXPRESSION TAG	UNP Q5Y7D3
D	201	GLY	-	EXPRESSION TAG	UNP Q5Y7D3
D	202	SER	-	EXPRESSION TAG	UNP Q5Y7D3
D	203	GLY	-	EXPRESSION TAG	UNP Q5Y7D3
D	204	GLY	-	EXPRESSION TAG	UNP Q5Y7D3
D	205	GLY	-	EXPRESSION TAG	UNP Q5Y7D3
D	206	SER	-	EXPRESSION TAG	UNP Q5Y7D3
D	207	CYS	-	EXPRESSION TAG	UNP Q5Y7D3
D	208	SER	-	EXPRESSION TAG	UNP Q5Y7D3
D	209	ARG	-	EXPRESSION TAG	UNP Q5Y7D3
D	210	GLY	-	EXPRESSION TAG	UNP Q5Y7D3
D	211	GLY	-	EXPRESSION TAG	UNP Q5Y7D3
D	212	LEU	-	EXPRESSION TAG	UNP Q5Y7D3
D	213	GLU	-	EXPRESSION TAG	UNP Q5Y7D3
D	214	VAL	-	EXPRESSION TAG	UNP Q5Y7D3
D	215	LEU	-	EXPRESSION TAG	UNP Q5Y7D3
D	216	PHE	-	EXPRESSION TAG	UNP Q5Y7D3
D	217	GLN	-	EXPRESSION TAG	UNP Q5Y7D3

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
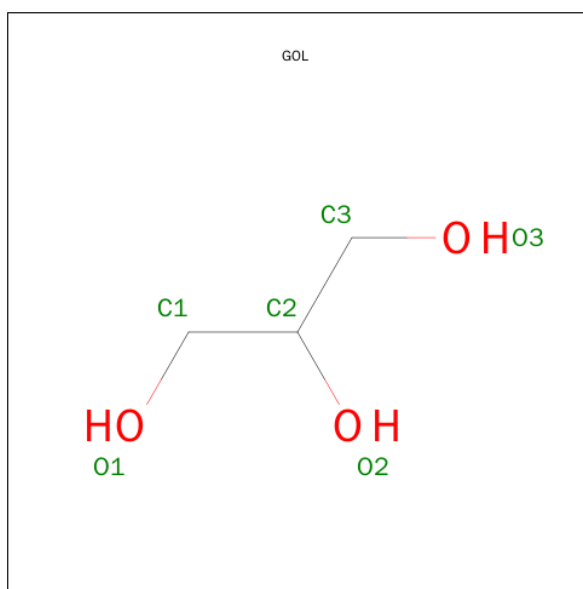
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	O 1	0	0
4	B	3	Total 3	O 3	0	0
4	C	1	Total 1	O 1	0	0
4	D	1	Total 1	O 1	0	0

# 3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.
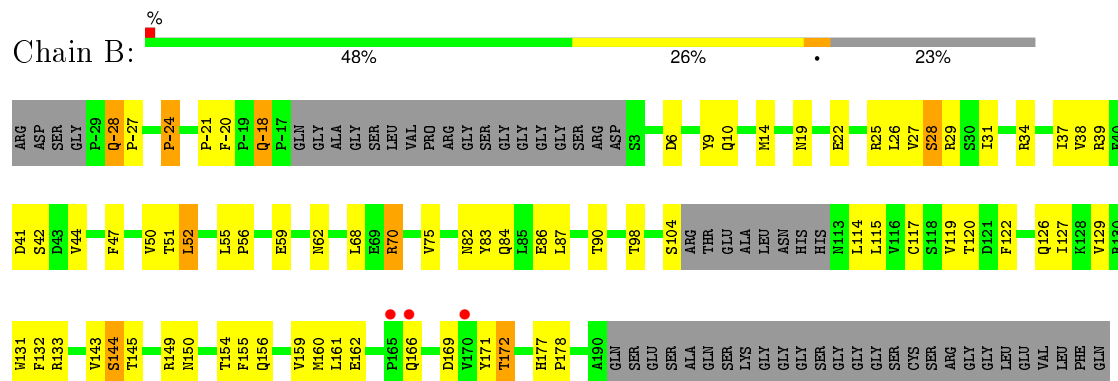
- Molecule 1: HLA-DQA1 protein
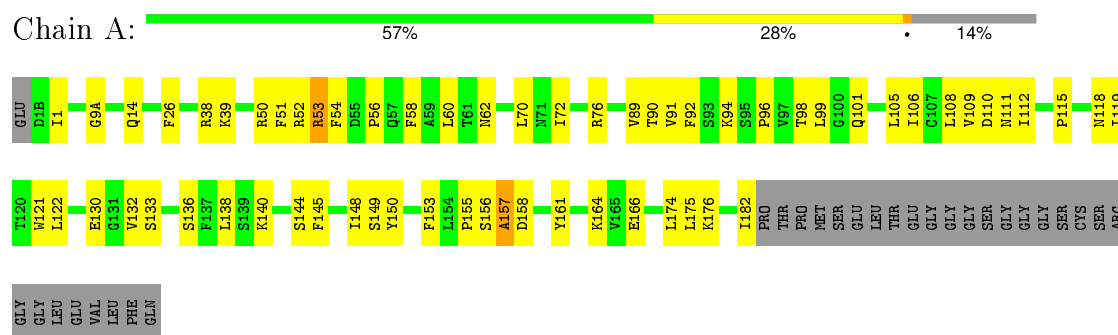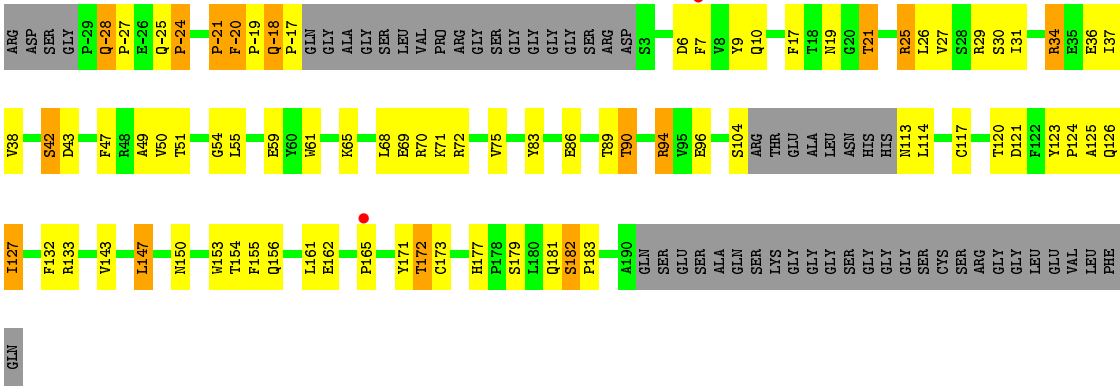

- Molecule 1: HLA-DQA1 protein
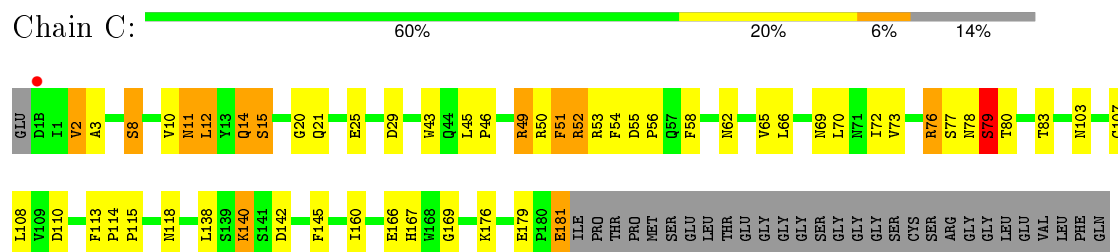
- Molecule 2: Peptide from Gamma-gliadin, linker, MHC class II antigen

- Molecule 2: Peptide from Gamma-gliadin, linker, MHC class II antigen

4   Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	74.89Å 114.92Å 138.03Å 90.00° 103.36° 90.00°	Depositor
Resolution (Å)	29.31 – 3.05 29.31 – 3.05	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.31-3.05) 99.9 (29.31-3.05)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.57 (at 3.05Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.210 , 0.283 0.215 , 0.286	Depositor DCC
R_{free} test set	1086 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	84.7	Xtriage
Anisotropy	0.166	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 62.3	EDS
Estimated twinning fraction	0.012 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Outliers	2 of 21712 reflections (0.009%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6120	wwPDB-VP
Average B, all atoms (Å^2)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.01% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.58	0/1518	0.68	0/2076
1	C	0.55	0/1517	0.67	0/2074
2	B	0.55	0/1615	0.70	1/2197 (0.0%)
2	D	0.52	0/1617	0.67	0/2198
All	All	0.55	0/6267	0.68	1/8545 (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
1	C	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	87	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	52	ARG	Peptide

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	1474	0	1394	40	0
1	C	1473	0	1395	45	0
2	B	1576	0	1530	57	0
2	D	1579	0	1532	60	0
3	A	6	0	8	0	0
3	B	6	0	8	1	0
4	A	1	0	0	0	0
4	B	3	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
All	All	6120	0	5867	170	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 14.

The worst 5 of 170 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:62:ASN:OD1	2:B:-21:PRO:HD2	1.64	0.97
2:B:59:GLU:OE1	2:D:162:GLU:HG2	1.76	0.84
1:A:53:ARG:HG3	1:A:54:PHE:H	1.44	0.83
2:D:133:ARG:HD3	2:D:171:TYR:HE1	1.49	0.78
1:C:53:ARG:HG3	1:C:54:PHE:H	1.49	0.76

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	182/213 (85%)	161 (88%)	17 (9%)	4 (2%)	8	34
1	C	181/213 (85%)	158 (87%)	19 (10%)	4 (2%)	8	34
2	B	187/250 (75%)	161 (86%)	23 (12%)	3 (2%)	12	42
2	D	187/250 (75%)	164 (88%)	18 (10%)	5 (3%)	6	28
All	All	737/926 (80%)	644 (87%)	77 (10%)	16 (2%)	8	34

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	-24	PRO
1	C	51	PHE
1	C	79	SER
2	D	121	ASP
1	C	2	VAL

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	166/190 (87%)	151 (91%)	15 (9%)	12	39
1	C	166/190 (87%)	146 (88%)	20 (12%)	6	23
2	B	176/216 (82%)	161 (92%)	15 (8%)	13	43
2	D	176/216 (82%)	154 (88%)	22 (12%)	6	21
All	All	684/812 (84%)	612 (90%)	72 (10%)	8	30

5 of 72 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	11	ASN
1	C	79	SER
2	D	143	VAL
1	C	12	LEU

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Mol	Chain	Res	Type
1	C	21	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	167	HIS
2	D	-28	GLN
2	D	134	ASN
2	B	156	GLN
2	D	84	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 ⓘ

2 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	$\#|Z| > 2$
3	GOL	A	301	-	5,5,5	0.37	0	5,5,5	1.10	1 (20%)
3	GOL	B	301	-	5,5,5	0.36	0	5,5,5	0.46	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
3	GOL	A	301	-	-	0/4/4/4	0/0/0/0
3	GOL	B	301	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	301	GOL	O2-C2-C1	2.01	117.86	108.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	301	GOL	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data (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, 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(Å²)	Q<0.9
1	A	184/213 (86%)	-0.32	0	100	100	50, 89, 112, 134	0
1	C	183/213 (85%)	-0.18	1 (0%)	91	81	67, 93, 116, 125	0
2	B	193/250 (77%)	-0.14	3 (1%)	74	52	53, 94, 121, 141	0
2	D	193/250 (77%)	-0.28	2 (1%)	84	66	67, 89, 118, 131	0
All	All	753/926 (81%)	-0.23	6 (0%)	87	72	50, 92, 118, 141	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	165	PRO	4.1
2	B	165	PRO	3.6
1	C	1(B)	ASP	2.6
2	B	170	VAL	2.3
2	D	7	PHE	2.3

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, 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	LLDF	B-factors(Å²)	Q<0.9
3	GOL	A	301	6/6	0.84	0.25	-	87,89,91,91	0
3	GOL	B	301	6/6	0.74	0.34	-	96,98,99,99	0

6.5   Other polymers (i)

There are no such residues in this entry.