wwPDB X-ray Structure Validation Summary Report (i)

May 6, 2024 – 04:09 PM EDT

PDB ID	:	8UAI
Title	:	Crystal structure of hetero hexameric hazelnut allergen Cor a 9
Authors	:	Zhang, Y.Z.; Guo, F.
Deposited on	:	2023-09-21
Resolution	:	1.92 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

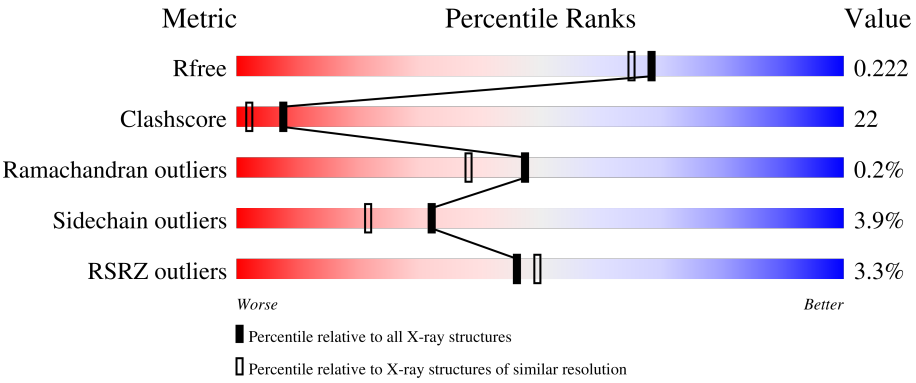
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 1.92 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	7937 (1.94-1.90)
Clashscore	141614	8644 (1.94-1.90)
Ramachandran outliers	138981	8530 (1.94-1.90)
Sidechain outliers	138945	8530 (1.94-1.90)
RSRZ outliers	127900	7793 (1.94-1.90)

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 >=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 <=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	493	3% 63% 18% • 17%
1	D	493	2% 60% 22% • 16%
2	B	494	3% 51% 25% • 22%
2	E	494	2% 54% 21% • 23%
3	C	493	3% 53% 29% • 16%

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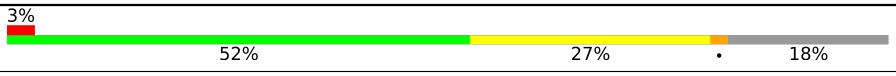
Mol	Chain	Length	Quality of chain
3	F	493	

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
4	GOL	C	502	-	-	X	-
4	GOL	E	505	-	-	X	-
5	CL	B	504	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 20351 atoms, of which 96 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 11S globulin 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	0	4	0
			3289	2024	628	633	4			
1	D	413	Total	C	N	O	S	0	10	0
			3397	2087	657	649	4			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ASP	ASN	conflict	UNP Q8W1C2
A	12	HIS	TYR	conflict	UNP Q8W1C2
A	35	GLY	CYS	conflict	UNP Q8W1C2
A	74	LYS	GLU	conflict	UNP Q8W1C2
A	144	ILE	CYS	conflict	UNP Q8W1C2
A	260	GLN	VAL	conflict	UNP Q8W1C2
A	314	GLY	CYS	conflict	UNP Q8W1C2
A	457	SER	GLU	conflict	UNP Q8W1C2
D	2	ASP	ASN	conflict	UNP Q8W1C2
D	12	HIS	TYR	conflict	UNP Q8W1C2
D	35	GLY	CYS	conflict	UNP Q8W1C2
D	74	LYS	GLU	conflict	UNP Q8W1C2
D	144	ILE	CYS	conflict	UNP Q8W1C2
D	260	GLN	VAL	conflict	UNP Q8W1C2
D	314	GLY	CYS	conflict	UNP Q8W1C2
D	457	SER	GLU	conflict	UNP Q8W1C2

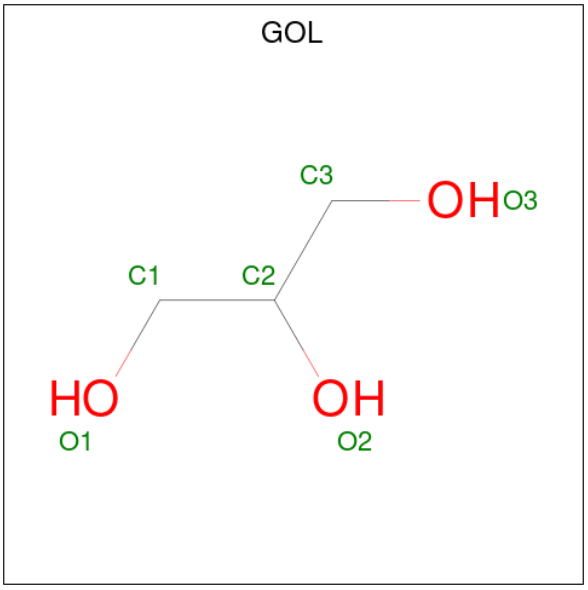
- Molecule 2 is a protein called 11S globulin 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	387	Total	C	N	O	S	0	12	0
			3146	1962	596	583	5			
2	E	382	Total	C	N	O	S	0	10	0
			3085	1926	576	578	5			

- Molecule 3 is a protein called 11S globulin 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	414	Total	C	N	O	S	0	18	0
			3375	2094	643	630	8			
3	F	402	Total	C	N	O	S	0	13	0
			3248	2018	610	612	8			

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O		0	0
			6	3	3			
4	A	1	Total	C	H	O	0	0
			14	3	8	3		
4	B	1	Total	C	O		0	0
			6	3	3			
4	B	1	Total	C	O		0	0
			6	3	3			
4	B	1	Total	C	H	O	0	0
			14	3	8	3		
4	C	1	Total	C	O		0	0
			6	3	3			
4	C	1	Total	C	H	O	0	0
			14	3	8	3		
4	D	1	Total	C	H	O	0	0
			14	3	8	3		
4	E	1	Total	C	H	O	0	0
			14	3	8	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	1	Total C H O 14 3 8 3	0	0
4	E	1	Total C H O 14 3 8 3	0	0
4	E	1	Total C H O 14 3 8 3	0	0
4	E	1	Total C H O 14 3 8 3	0	0
4	F	1	Total C H O 14 3 8 3	0	0
4	F	1	Total C H O 14 3 8 3	0	0
4	F	1	Total C H O 14 3 8 3	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Cl 1 1	0	0
5	D	1	Total Cl 1 1	0	0

- Molecule 6 is water.

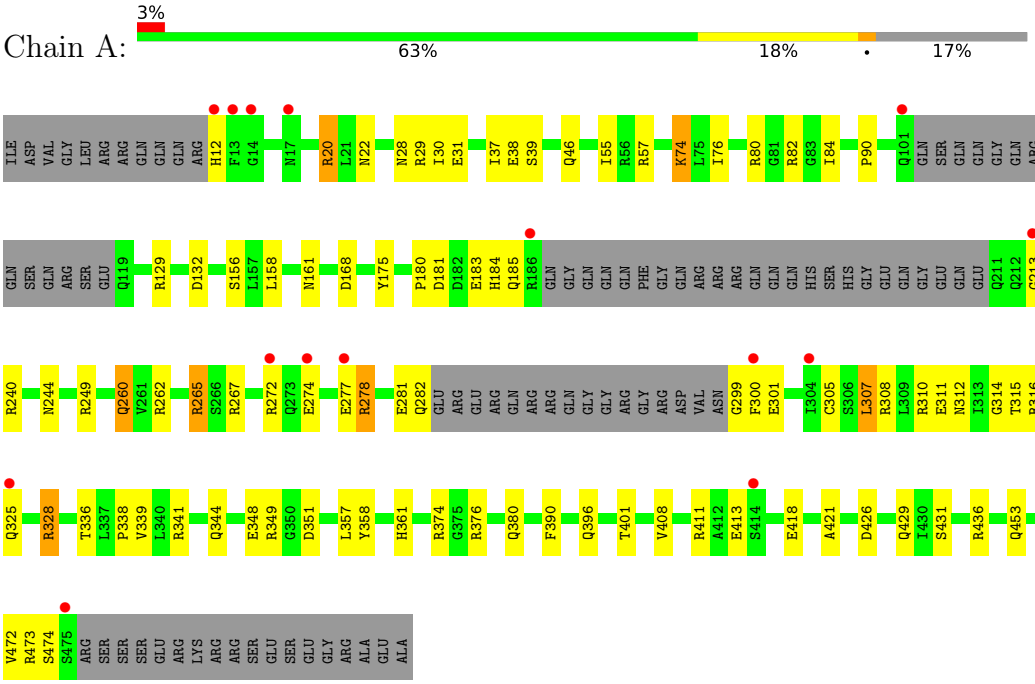
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	91	Total O 91 91	0	0
6	B	95	Total O 95 95	0	0
6	C	110	Total O 110 110	0	0
6	D	125	Total O 125 125	0	0
6	E	97	Total O 97 97	0	0
6	F	99	Total O 99 99	0	0

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.

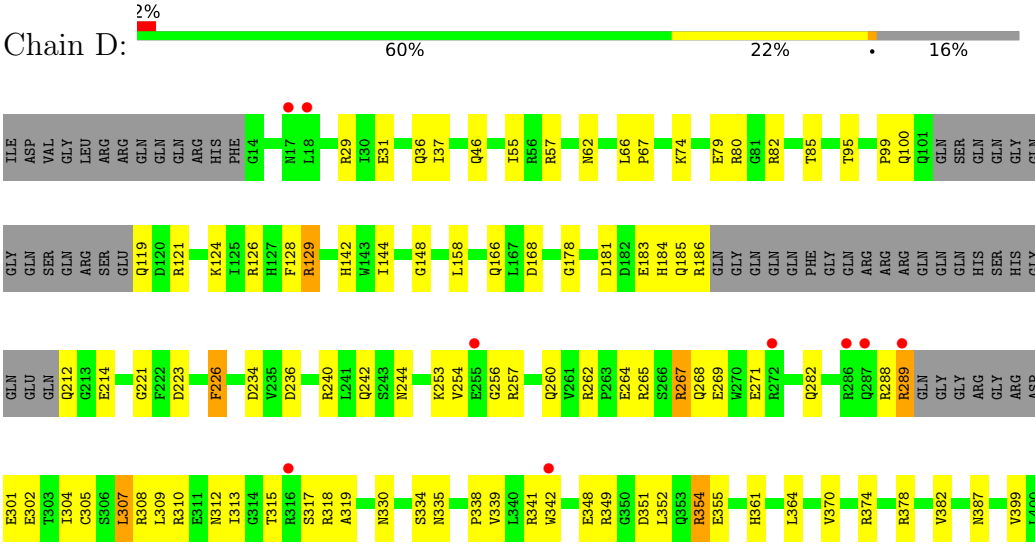
- Molecule 1: 11S globulin 1

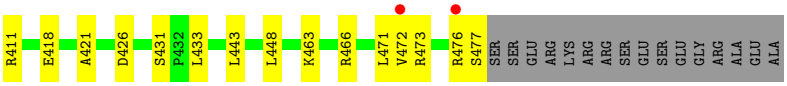
Chain A:



- Molecule 1: 11S globulin 1

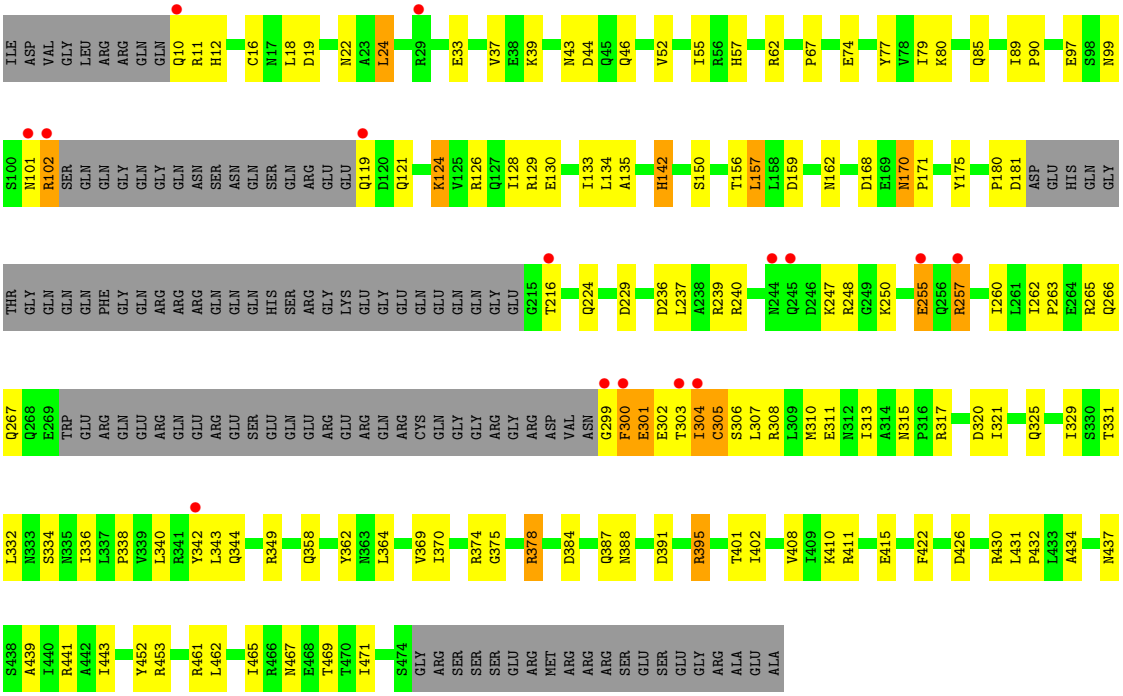
Chain D:





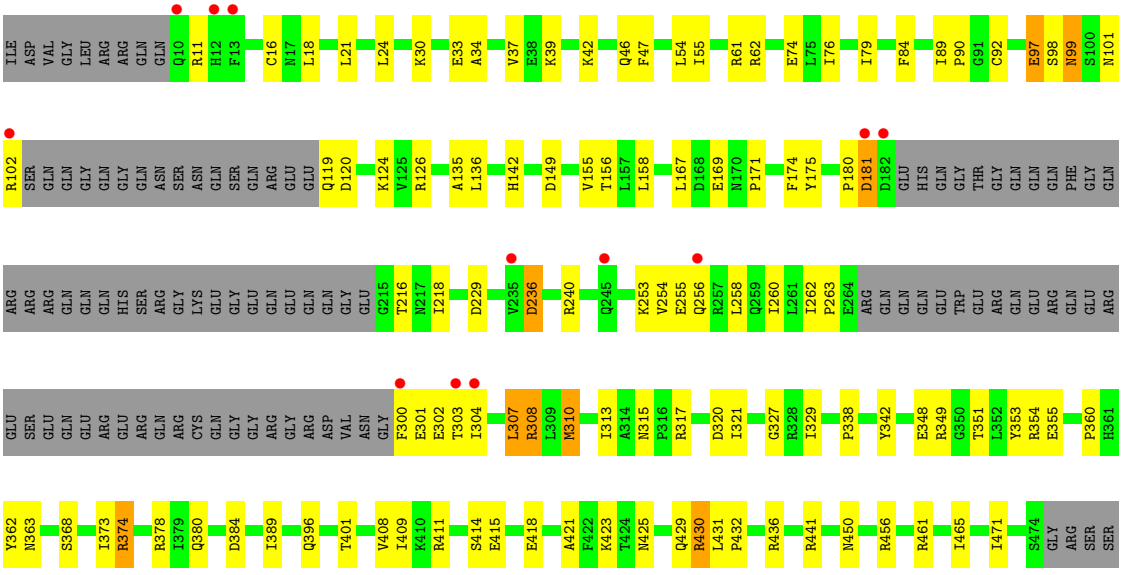
• Molecule 2: 11S globulin 2

Chain B:



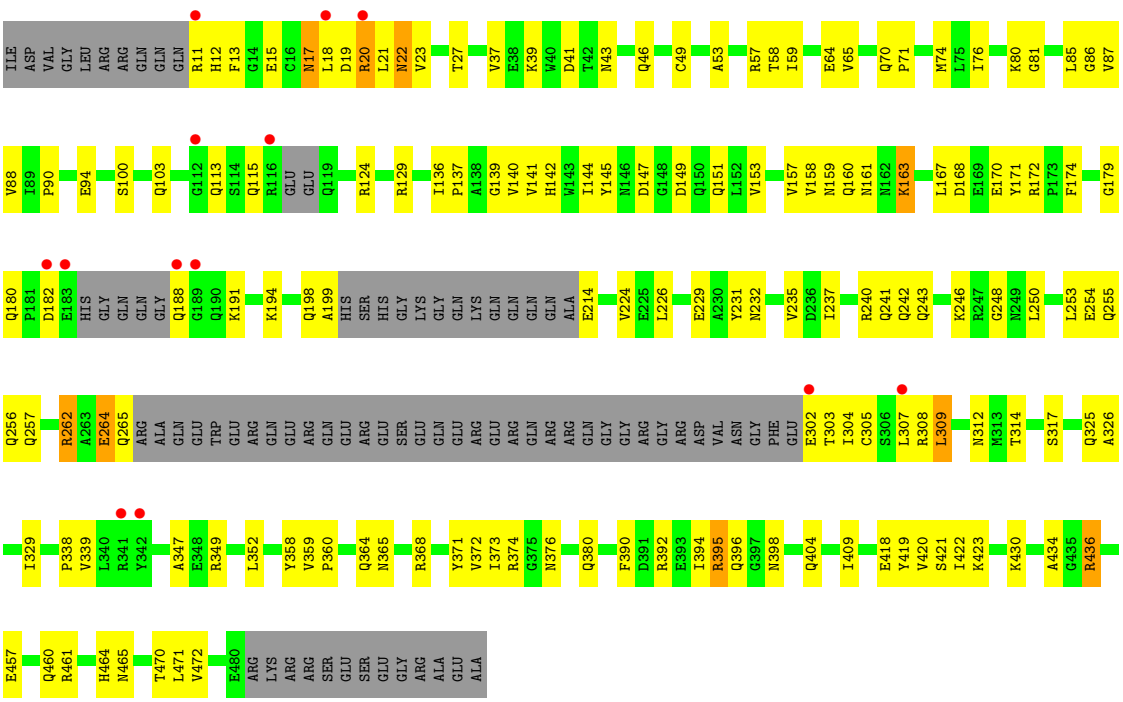
• Molecule 2: 11S globulin 2

Chain E:



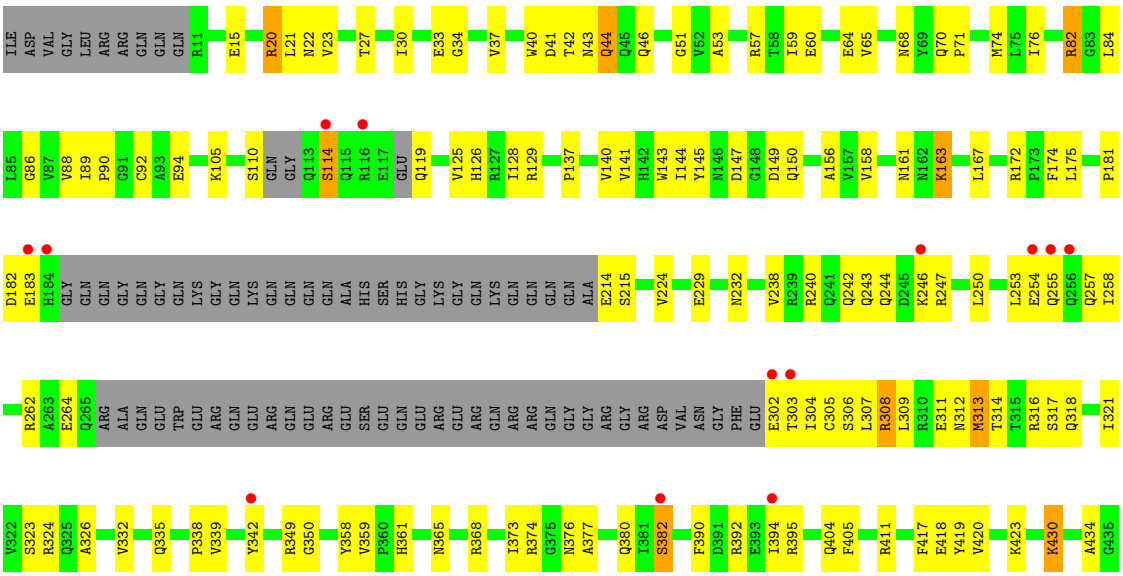
- Molecule 3: 11S globulin 3

Chain C:



- Molecule 3: 11S globulin 3

Chain F:




R436
T437
S438
R441
N465
R466
T470
L471
S479
E480
ARG
LYS
ARG
ARG
SER
GLU
SER
GLU
GLY
ARG
ALA
GLU
ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	149.17Å 91.09Å 74.85Å 90.00° 90.32° 90.00°	Depositor
Resolution (Å)	45.80 – 1.92 45.80 – 1.92	Depositor EDS
% Data completeness (in resolution range)	92.6 (45.80-1.92) 92.6 (45.80-1.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.89 (at 1.92Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.174 , 0.221 0.174 , 0.222	Depositor DCC
R_{free} test set	7119 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	31.7	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 55.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	20351	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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, CL

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	0.41	0/3360	0.67	0/4550
1	D	0.42	0/3485	0.70	0/4712
2	B	0.43	0/3231	0.68	0/4355
2	E	0.40	0/3161	0.66	0/4266
3	C	0.43	0/3475	0.67	0/4690
3	F	0.44	0/3337	0.69	0/4509
All	All	0.42	0/20049	0.68	0/27082

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
2	E	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	374	ARG	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	3289	0	3158	90	0
1	D	3397	0	3302	138	0
2	B	3146	0	3151	189	0
2	E	3085	0	3072	144	1
3	C	3375	0	3385	205	0
3	F	3248	0	3223	193	0
4	A	12	8	16	2	0
4	B	18	8	24	1	0
4	C	12	8	16	7	0
4	D	6	8	8	1	0
4	E	30	40	40	7	0
4	F	18	24	24	0	0
5	B	1	0	0	3	0
5	D	1	0	0	0	0
6	A	91	0	0	1	0
6	B	95	0	0	9	0
6	C	110	0	0	10	0
6	D	125	0	0	8	0
6	E	97	0	0	3	0
6	F	99	0	0	5	0
All	All	20255	96	19419	856	1

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 22.

The worst 5 of 856 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)
3:C:436[B]:ARG:HB3	3:C:470:THR:HG22	1.32	1.09
1:D:466:ARG:CZ	1:D:472:VAL:HG21	1.86	1.05
3:C:304:ILE:HG13	3:C:307[B]:LEU:HD11	1.43	1.01
2:B:99:ASN:HD21	1:D:473:ARG:HE	1.07	0.98
3:C:65:VAL:HG22	3:C:144:ILE:H	1.29	0.97

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:415:GLU:OE2	2:E:456:ARG:NH2[2_655]	2.17	0.03

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	403/493 (82%)	390 (97%)	12 (3%)	1 (0%)	47	38
1	D	415/493 (84%)	402 (97%)	12 (3%)	1 (0%)	47	38
2	B	391/494 (79%)	376 (96%)	14 (4%)	1 (0%)	41	31
2	E	384/494 (78%)	369 (96%)	14 (4%)	1 (0%)	41	31
3	C	422/493 (86%)	406 (96%)	16 (4%)	0	100	100
3	F	405/493 (82%)	391 (96%)	13 (3%)	1 (0%)	47	38
All	All	2420/2960 (82%)	2334 (96%)	81 (3%)	5 (0%)	47	38

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	305	CYS
3	F	114	SER
1	A	307	LEU
1	D	307	LEU
2	E	167	LEU

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	350/422 (83%)	336 (96%)	14 (4%)	31	21
1	D	365/422 (86%)	356 (98%)	9 (2%)	47	39
2	B	338/422 (80%)	317 (94%)	21 (6%)	18	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	E	332/422 (79%)	319 (96%)	13 (4%)	32 22
3	C	368/420 (88%)	347 (94%)	21 (6%)	20 10
3	F	353/420 (84%)	341 (97%)	12 (3%)	37 27
All	All	2106/2528 (83%)	2016 (96%)	90 (4%)	32 18

5 of 90 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	129[B]	ARG
2	E	181	ASP
1	D	257	ARG
2	E	11	ARG
2	E	310	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	330	ASN
3	F	46	GLN
2	E	429	GLN
3	F	70	GLN
2	B	170	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 for Mogul analysis.

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	$\#\|Z\| > 2$
4	GOL	E	501	-	5,5,5	0.85	0	5,5,5	1.10	1 (20%)
4	GOL	E	505	-	5,5,5	0.91	0	5,5,5	1.17	1 (20%)
4	GOL	B	501	-	5,5,5	0.71	0	5,5,5	1.20	1 (20%)
4	GOL	A	501	-	5,5,5	0.79	0	5,5,5	1.16	0
4	GOL	E	502	-	5,5,5	0.65	0	5,5,5	0.83	0
4	GOL	F	503	-	5,5,5	0.83	0	5,5,5	1.04	0
4	GOL	D	502	-	5,5,5	0.79	0	5,5,5	0.93	0
4	GOL	E	504	-	5,5,5	1.10	0	5,5,5	1.23	1 (20%)
4	GOL	F	501	-	5,5,5	0.86	0	5,5,5	0.93	0
4	GOL	C	501	-	5,5,5	0.70	0	5,5,5	1.09	0
4	GOL	E	503	-	5,5,5	0.52	0	5,5,5	0.63	0
4	GOL	F	502	-	5,5,5	0.95	0	5,5,5	1.03	0
4	GOL	B	503	-	5,5,5	0.92	0	5,5,5	1.22	1 (20%)
4	GOL	B	502	-	5,5,5	1.11	0	5,5,5	1.00	0
4	GOL	A	502	-	5,5,5	0.94	0	5,5,5	1.26	1 (20%)
4	GOL	C	502	-	5,5,5	1.07	0	5,5,5	1.06	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
4	GOL	E	501	-	-	2/4/4/4	-
4	GOL	E	505	-	-	0/4/4/4	-
4	GOL	B	501	-	-	2/4/4/4	-
4	GOL	A	501	-	-	3/4/4/4	-
4	GOL	E	502	-	-	2/4/4/4	-
4	GOL	F	503	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	D	502	-	-	2/4/4/4	-
4	GOL	E	504	-	-	2/4/4/4	-
4	GOL	F	501	-	-	2/4/4/4	-
4	GOL	C	501	-	-	2/4/4/4	-
4	GOL	E	503	-	-	2/4/4/4	-
4	GOL	F	502	-	-	0/4/4/4	-
4	GOL	B	503	-	-	0/4/4/4	-
4	GOL	B	502	-	-	0/4/4/4	-
4	GOL	A	502	-	-	4/4/4/4	-
4	GOL	C	502	-	-	0/4/4/4	-

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	503	GOL	C3-C2-C1	-2.42	102.31	111.70
4	A	502	GOL	C3-C2-C1	-2.42	102.31	111.70
4	E	504	GOL	C3-C2-C1	-2.38	102.46	111.70
4	E	505	GOL	C3-C2-C1	-2.25	102.94	111.70
4	B	501	GOL	C3-C2-C1	-2.06	103.69	111.70

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	501	GOL	O2-C2-C3-O3
4	A	502	GOL	O1-C1-C2-C3
4	A	502	GOL	C1-C2-C3-O3
4	B	501	GOL	C1-C2-C3-O3
4	C	501	GOL	C1-C2-C3-O3

There are no ring outliers.

7 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	501	GOL	1	0
4	E	505	GOL	6	0
4	A	501	GOL	2	0
4	D	502	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	501	GOL	3	0
4	B	502	GOL	1	0
4	C	502	GOL	4	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^{th} 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	407/493 (82%)	0.15	15 (3%)	41	44	26, 36, 58, 72	0
1	D	413/493 (83%)	0.08	12 (2%)	51	55	24, 35, 58, 85	0
2	B	387/494 (78%)	0.12	15 (3%)	39	42	25, 34, 55, 76	0
2	E	382/494 (77%)	0.10	12 (3%)	49	52	26, 37, 58, 77	0
3	C	414/493 (83%)	0.14	13 (3%)	49	52	25, 35, 56, 77	0
3	F	402/493 (81%)	0.12	13 (3%)	47	50	24, 34, 55, 82	0
All	All	2405/2960 (81%)	0.12	80 (3%)	46	49	24, 35, 57, 85	0

The worst 5 of 80 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	182	ASP	4.9
2	E	300	PHE	4.8
2	E	13	PHE	4.7
3	C	116	ARG	4.7
1	D	300	PHE	4.7

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

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^{th} 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
4	GOL	E	501	6/6	0.62	0.21	60,73,86,86	0
4	GOL	B	503	6/6	0.63	0.25	59,75,86,91	0
4	GOL	F	502	6/6	0.68	0.20	73,88,97,97	0
4	GOL	C	502	6/6	0.71	0.18	54,65,72,73	0
4	GOL	A	501	6/6	0.73	0.24	53,58,61,74	0
4	GOL	A	502	6/6	0.74	0.21	66,80,85,85	0
4	GOL	E	503	6/6	0.76	0.15	57,69,82,82	0
4	GOL	E	504	6/6	0.77	0.28	58,69,84,84	0
4	GOL	D	502	6/6	0.77	0.23	46,58,69,69	0
4	GOL	F	503	6/6	0.78	0.17	74,89,98,100	0
4	GOL	C	501	6/6	0.82	0.23	47,50,53,57	0
4	GOL	B	502	6/6	0.83	0.25	39,45,49,52	0
4	GOL	E	502	6/6	0.83	0.13	44,57,68,71	0
4	GOL	F	501	6/6	0.90	0.12	48,60,72,72	0
4	GOL	B	501	6/6	0.90	0.17	43,47,50,53	0
4	GOL	E	505	6/6	0.90	0.19	42,51,59,62	0
5	CL	B	504	1/1	0.98	0.05	46,46,46,46	0
5	CL	D	501	1/1	0.98	0.07	37,37,37,37	0

6.5 Other polymers (i)

There are no such residues in this entry.