wwPDB X-ray Structure Validation Summary Report (i)

Jun 23, 2024 – 05:51 PM EDT

PDB ID	:	5C4V
Title	:	Ski-like protein
Authors	:	Wallden, K.; Nyman, T.; Hallberg, B.M.
Deposited on	:	2015-06-18
Resolution	:	2.60 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 (i)) were used in the production of this report:

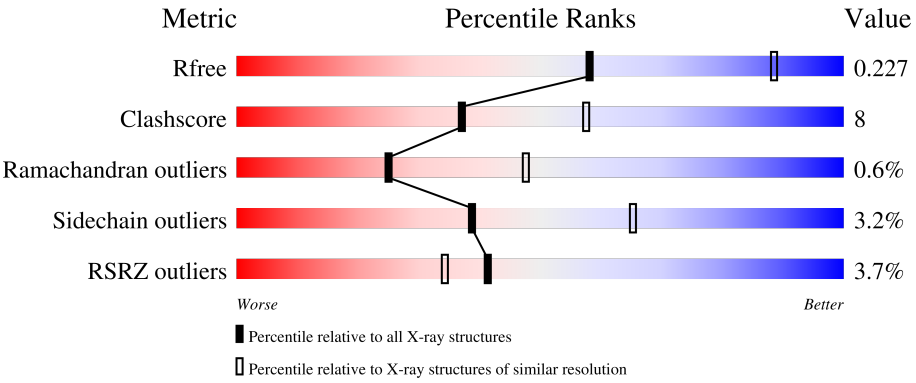
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	258	65% 9% 26%
1	C	258	62% 10% 27%
1	E	258	68% 7% 24%
2	B	127	64% 9% 24%
2	D	127	5% 65% 6% 28%

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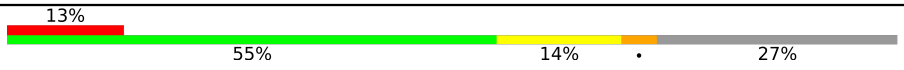
Mol	Chain	Length	Quality of chain
2	F	127	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6835 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 Mothers against decapentaplegic homolog 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	192	Total	C	N	O	S	0	1	0
			1517	961	271	274	11			
1	C	188	Total	C	N	O	S	0	0	0
			1496	948	266	271	11			
1	E	196	Total	C	N	O	S	0	0	0
			1543	976	279	277	11			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	292	MET	-	initiating methionine	UNP Q13485
A	293	HIS	-	expression tag	UNP Q13485
A	294	HIS	-	expression tag	UNP Q13485
A	295	HIS	-	expression tag	UNP Q13485
A	296	HIS	-	expression tag	UNP Q13485
A	297	HIS	-	expression tag	UNP Q13485
A	298	HIS	-	expression tag	UNP Q13485
A	299	SER	-	expression tag	UNP Q13485
A	300	SER	-	expression tag	UNP Q13485
A	301	GLY	-	expression tag	UNP Q13485
A	302	VAL	-	expression tag	UNP Q13485
A	303	ASP	-	expression tag	UNP Q13485
A	304	LEU	-	expression tag	UNP Q13485
A	305	GLY	-	expression tag	UNP Q13485
A	306	THR	-	expression tag	UNP Q13485
A	307	GLU	-	expression tag	UNP Q13485
A	308	ASN	-	expression tag	UNP Q13485
A	309	LEU	-	expression tag	UNP Q13485
A	310	TYR	-	expression tag	UNP Q13485
A	311	PHE	-	expression tag	UNP Q13485
A	312	GLN	-	expression tag	UNP Q13485
A	313	SER	-	expression tag	UNP Q13485
C	292	MET	-	initiating methionine	UNP Q13485

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Chain	Residue	Modelled	Actual	Comment	Reference
C	293	HIS	-	expression tag	UNP Q13485
C	294	HIS	-	expression tag	UNP Q13485
C	295	HIS	-	expression tag	UNP Q13485
C	296	HIS	-	expression tag	UNP Q13485
C	297	HIS	-	expression tag	UNP Q13485
C	298	HIS	-	expression tag	UNP Q13485
C	299	SER	-	expression tag	UNP Q13485
C	300	SER	-	expression tag	UNP Q13485
C	301	GLY	-	expression tag	UNP Q13485
C	302	VAL	-	expression tag	UNP Q13485
C	303	ASP	-	expression tag	UNP Q13485
C	304	LEU	-	expression tag	UNP Q13485
C	305	GLY	-	expression tag	UNP Q13485
C	306	THR	-	expression tag	UNP Q13485
C	307	GLU	-	expression tag	UNP Q13485
C	308	ASN	-	expression tag	UNP Q13485
C	309	LEU	-	expression tag	UNP Q13485
C	310	TYR	-	expression tag	UNP Q13485
C	311	PHE	-	expression tag	UNP Q13485
C	312	GLN	-	expression tag	UNP Q13485
C	313	SER	-	expression tag	UNP Q13485
E	292	MET	-	initiating methionine	UNP Q13485
E	293	HIS	-	expression tag	UNP Q13485
E	294	HIS	-	expression tag	UNP Q13485
E	295	HIS	-	expression tag	UNP Q13485
E	296	HIS	-	expression tag	UNP Q13485
E	297	HIS	-	expression tag	UNP Q13485
E	298	HIS	-	expression tag	UNP Q13485
E	299	SER	-	expression tag	UNP Q13485
E	300	SER	-	expression tag	UNP Q13485
E	301	GLY	-	expression tag	UNP Q13485
E	302	VAL	-	expression tag	UNP Q13485
E	303	ASP	-	expression tag	UNP Q13485
E	304	LEU	-	expression tag	UNP Q13485
E	305	GLY	-	expression tag	UNP Q13485
E	306	THR	-	expression tag	UNP Q13485
E	307	GLU	-	expression tag	UNP Q13485
E	308	ASN	-	expression tag	UNP Q13485
E	309	LEU	-	expression tag	UNP Q13485
E	310	TYR	-	expression tag	UNP Q13485
E	311	PHE	-	expression tag	UNP Q13485
E	312	GLN	-	expression tag	UNP Q13485

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Chain	Residue	Modelled	Actual	Comment	Reference
E	313	SER	-	expression tag	UNP Q13485

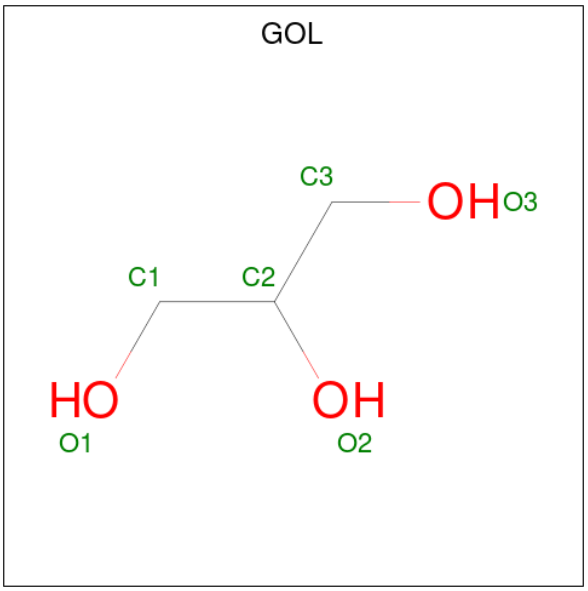
- Molecule 2 is a protein called Ski-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	96	Total	C	N	O	S	0	0	0
			743	478	128	126	11			
2	D	91	Total	C	N	O	S	0	0	0
			697	448	118	120	11			
2	F	93	Total	C	N	O	S	0	0	0
			698	445	118	125	10			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	237	MET	-	initiating methionine	UNP P12757
B	357	ALA	-	expression tag	UNP P12757
B	358	HIS	-	expression tag	UNP P12757
B	359	HIS	-	expression tag	UNP P12757
B	360	HIS	-	expression tag	UNP P12757
B	361	HIS	-	expression tag	UNP P12757
B	362	HIS	-	expression tag	UNP P12757
B	363	HIS	-	expression tag	UNP P12757
D	237	MET	-	initiating methionine	UNP P12757
D	357	ALA	-	expression tag	UNP P12757
D	358	HIS	-	expression tag	UNP P12757
D	359	HIS	-	expression tag	UNP P12757
D	360	HIS	-	expression tag	UNP P12757
D	361	HIS	-	expression tag	UNP P12757
D	362	HIS	-	expression tag	UNP P12757
D	363	HIS	-	expression tag	UNP P12757
F	237	MET	-	initiating methionine	UNP P12757
F	357	ALA	-	expression tag	UNP P12757
F	358	HIS	-	expression tag	UNP P12757
F	359	HIS	-	expression tag	UNP P12757
F	360	HIS	-	expression tag	UNP P12757
F	361	HIS	-	expression tag	UNP P12757
F	362	HIS	-	expression tag	UNP P12757
F	363	HIS	-	expression tag	UNP P12757

- 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 6 3 3	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Zn 1 1	0	0
4	D	1	Total Zn 1 1	0	0
4	F	1	Total Zn 1 1	0	0

- Molecule 5 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	2	Total Ni 2 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	41	Total O 41 41	0	0
6	C	32	Total O 32 32	0	0

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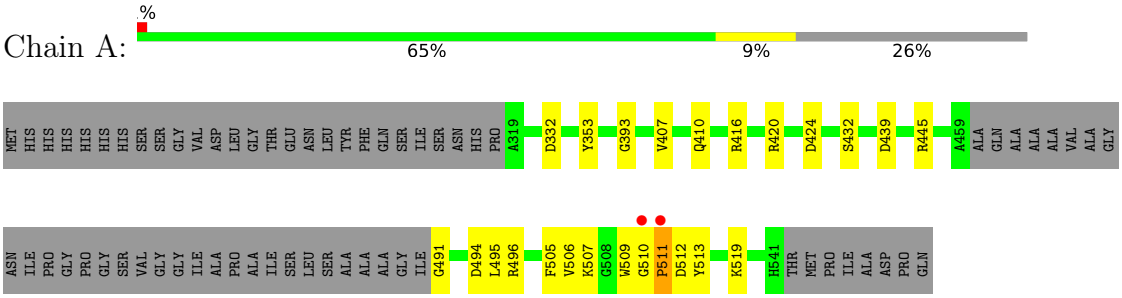
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	E	39	Total O 39 39	0	0
6	B	10	Total O 10 10	0	0
6	D	4	Total O 4 4	0	0
6	F	4	Total O 4 4	0	0

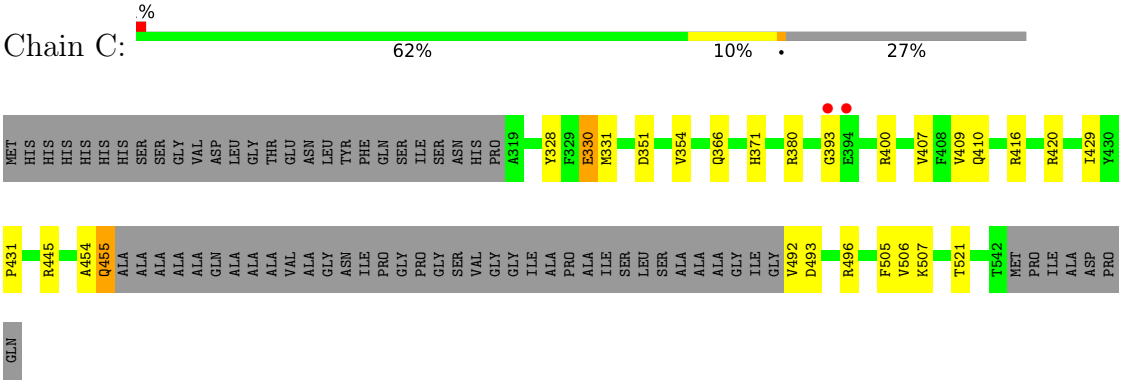
3 Residue-property plots (i)

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.

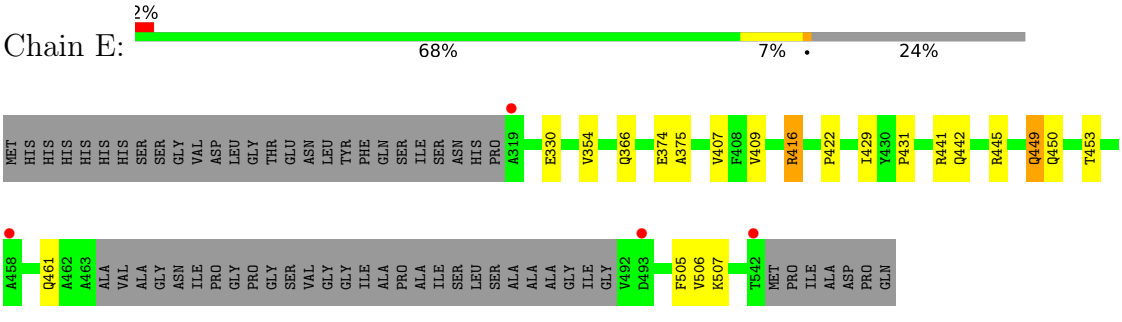
• Molecule 1: Mothers against decapentaplegic homolog 4



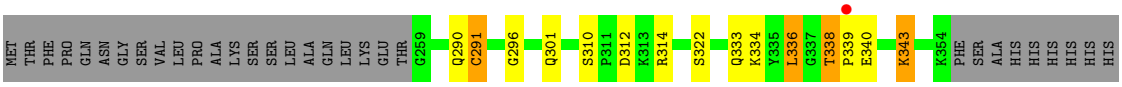
• Molecule 1: Mothers against decapentaplegic homolog 4



• Molecule 1: Mothers against decapentaplegic homolog 4

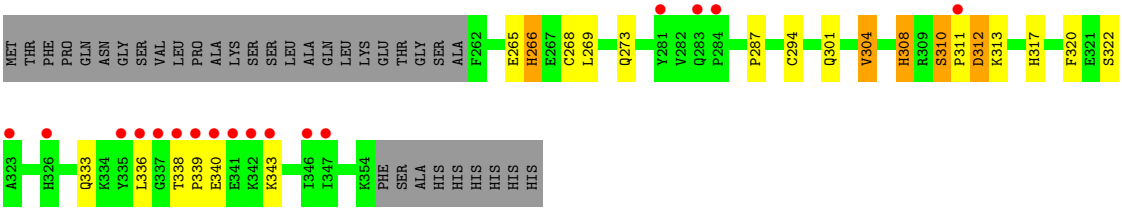


• Molecule 2: Ski-like protein



• Molecule 2: Ski-like protein

• Molecule 2: Ski-like protein



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	213.54Å 122.83Å 51.57Å 90.00° 90.72° 90.00°	Depositor
Resolution (Å)	40.30 – 2.60 40.34 – 2.57	Depositor EDS
% Data completeness (in resolution range)	93.8 (40.30-2.60) 96.9 (40.34-2.57)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.49 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.8.0123	Depositor
R, R_{free}	0.208 , 0.242 0.192 , 0.227	Depositor DCC
R_{free} test set	1735 reflections (4.23%)	wwPDB-VP
Wilson B-factor (Å^2)	37.8	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 57.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.005 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.000 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.001 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.000 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.021 for -h,-k,l	Xtriage
Reported twinning fraction	0.835 for H, K, L 0.165 for -1/2H+3/2K, -1/2H-1/2K, L	Depositor
Outliers	0 of 41039 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6835	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.95% 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: ZN, GOL, NI

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	1.05	0/1557	1.08	6/2111 (0.3%)
1	C	0.96	2/1533 (0.1%)	0.99	6/2078 (0.3%)
1	E	1.08	2/1580 (0.1%)	1.01	4/2142 (0.2%)
2	B	0.87	1/767 (0.1%)	0.91	1/1038 (0.1%)
2	D	0.72	0/720	0.81	0/979
2	F	0.75	0/722	0.88	1/984 (0.1%)
All	All	0.96	5/6879 (0.1%)	0.98	18/9332 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	330	GLU	CD-OE2	-6.28	1.18	1.25
1	E	330	GLU	CD-OE2	-5.91	1.19	1.25
1	E	330	GLU	CD-OE1	-5.77	1.19	1.25
1	C	330	GLU	CD-OE1	-5.23	1.19	1.25
2	B	291	CYS	CB-SG	5.18	1.91	1.82

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	291	CYS	CA-CB-SG	14.57	140.23	114.00
1	C	420	ARG	NE-CZ-NH2	-7.41	116.59	120.30
1	A	439	ASP	CB-CG-OD1	7.39	124.95	118.30
1	E	416	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	C	420	ARG	CG-CD-NE	-6.50	98.16	111.80

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	1517	0	1472	37	0
1	C	1496	0	1447	17	0
1	E	1543	0	1501	13	0
2	B	743	0	689	15	0
2	D	697	0	630	6	0
2	F	698	0	586	21	0
3	A	6	0	8	2	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
5	B	2	0	0	0	0
6	A	41	0	0	4	0
6	B	10	0	0	0	0
6	C	32	0	0	2	0
6	D	4	0	0	0	0
6	E	39	0	0	0	0
6	F	4	0	0	0	0
All	All	6835	0	6333	101	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 8.

The worst 5 of 101 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:491:GLY:O	1:A:495:LEU:N	1.81	1.13
2:B:333:GLN:HA	2:B:336:LEU:HD12	1.42	1.02
1:A:491:GLY:CA	1:A:494:ASP:OD2	2.09	1.00
1:A:510:GLY:H	1:A:513:TYR:HB2	1.23	0.99
1:A:491:GLY:O	1:A:494:ASP:N	1.97	0.97

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	189/258 (73%)	180 (95%)	8 (4%)	1 (0%)	29 52
1	C	184/258 (71%)	174 (95%)	9 (5%)	1 (0%)	29 52
1	E	192/258 (74%)	183 (95%)	9 (5%)	0	100 100
2	B	94/127 (74%)	90 (96%)	4 (4%)	0	100 100
2	D	89/127 (70%)	85 (96%)	3 (3%)	1 (1%)	14 30
2	F	91/127 (72%)	88 (97%)	1 (1%)	2 (2%)	6 12
All	All	839/1155 (73%)	800 (95%)	34 (4%)	5 (1%)	25 47

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	393	GLY
2	F	310	SER
1	A	393	GLY
2	D	287	PRO
2	F	287	PRO

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	159/208 (76%)	157 (99%)	2 (1%)	69 86
1	C	159/208 (76%)	157 (99%)	2 (1%)	69 86
1	E	160/208 (77%)	157 (98%)	3 (2%)	57 79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	76/112 (68%)	70 (92%)	6 (8%)	12 24
2	D	71/112 (63%)	66 (93%)	5 (7%)	15 30
2	F	66/112 (59%)	62 (94%)	4 (6%)	18 38
All	All	691/960 (72%)	669 (97%)	22 (3%)	39 65

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	267	GLU
2	D	336	LEU
2	D	334	LYS
2	F	266	HIS
1	E	449	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	326	HIS
2	F	266	HIS
2	F	326	HIS
2	D	266	HIS
2	B	266	HIS

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 6 ligands modelled in this entry, 5 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
3	GOL	A	601	-	5,5,5	0.98	0	5,5,5	1.10	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	601	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	GOL	O1-C1-C2-O2
3	A	601	GOL	O1-C1-C2-C3
3	A	601	GOL	O2-C2-C3-O3
3	A	601	GOL	C1-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	GOL	2	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	192/258 (74%)	-0.34	2 (1%)	82	80	12, 27, 60, 102	0
1	C	188/258 (72%)	-0.18	2 (1%)	80	78	14, 33, 57, 83	0
1	E	196/258 (75%)	-0.32	4 (2%)	65	60	12, 30, 63, 86	0
2	B	96/127 (75%)	-0.08	1 (1%)	82	80	20, 45, 73, 106	0
2	D	91/127 (71%)	0.38	6 (6%)	18	13	29, 58, 90, 119	0
2	F	93/127 (73%)	0.75	17 (18%)	1	0	26, 63, 109, 122	0
All	All	856/1155 (74%)	-0.08	32 (3%)	41	34	12, 37, 80, 122	0

The worst 5 of 32 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	337	GLY	5.5
2	F	335	TYR	5.3
2	D	284	PRO	5.2
2	D	337	GLY	4.8
2	F	339	PRO	4.8

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
3	GOL	A	601	6/6	0.83	0.20	31,36,44,44	0
5	NI	B	402	1/1	0.92	0.15	86,86,86,86	0
5	NI	B	403	1/1	0.96	0.22	98,98,98,98	0
4	ZN	B	401	1/1	0.98	0.06	48,48,48,48	0
4	ZN	D	401	1/1	0.99	0.03	57,57,57,57	0
4	ZN	F	401	1/1	0.99	0.04	41,41,41,41	0

6.5 Other polymers (i)

There are no such residues in this entry.