



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 01:02 am GMT

PDB ID : 2OAX
Title : Crystal structure of the S810L mutant mineralocorticoid receptor associated with SC9420
Authors : Huyet, J.; Pinon, G.M.; Fay, M.R.; Rafestin-Oblin, M.E.; Fagart, J.
Deposited on : 2006-12-18
Resolution : 2.29 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

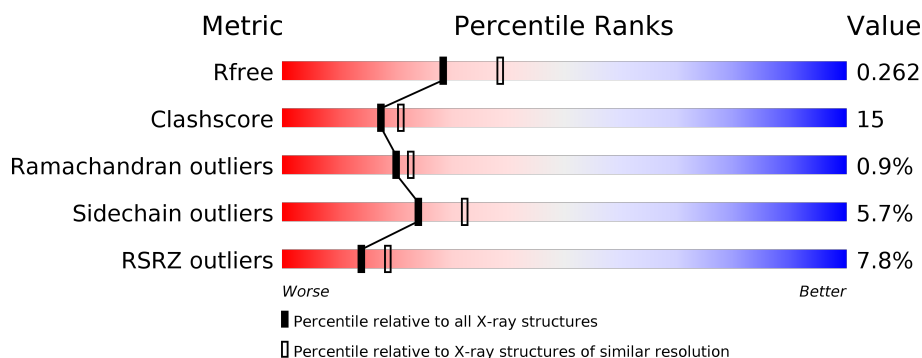
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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 $\leq 5\%$. 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	256	<div> <div>8%</div> <div> <div></div> <div>62%</div> <div>27%</div> <div>•</div> <div>9%</div> </div> </div>
1	B	256	<div> <div>4%</div> <div> <div></div> <div>62%</div> <div>26%</div> <div>•</div> <div>9%</div> </div> </div>
1	C	256	<div> <div>3%</div> <div> <div></div> <div>68%</div> <div>22%</div> <div>•</div> <div>9%</div> </div> </div>
1	D	256	<div> <div>7%</div> <div> <div></div> <div>64%</div> <div>26%</div> <div>•</div> <div>9%</div> </div> </div>
1	E	256	<div> <div>14%</div> <div> <div></div> <div>53%</div> <div>36%</div> <div>•</div> <div>9%</div> </div> </div>
1	F	256	<div> <div>7%</div> <div> <div></div> <div>66%</div> <div>25%</div> <div>•</div> <div>7%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12016 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 Mineralocorticoid receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	233	Total	C	N	O	S	0	0	0
			1903	1242	303	344	14			
1	B	233	Total	C	N	O	S	0	0	0
			1916	1248	307	347	14			
1	C	233	Total	C	N	O	S	0	0	0
			1913	1246	306	347	14			
1	D	234	Total	C	N	O	S	0	0	0
			1919	1250	308	347	14			
1	E	234	Total	C	N	O	S	0	0	0
			1912	1244	307	347	14			
1	F	238	Total	C	N	O	S	0	0	0
			1940	1261	311	354	14			

There are 24 discrepancies between the modelled and reference sequences:

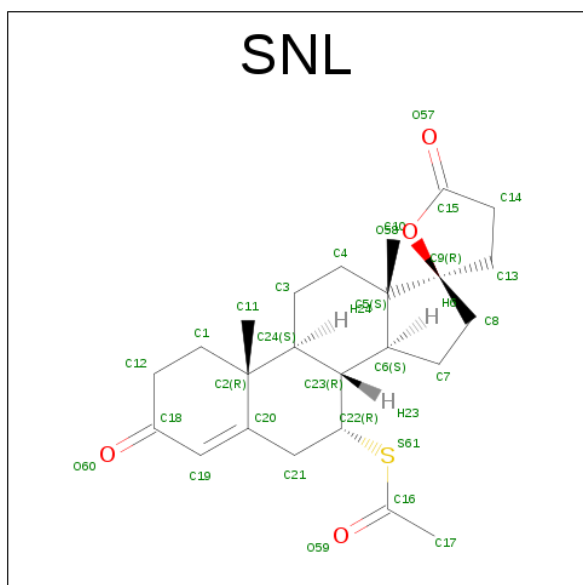
Chain	Residue	Modelled	Actual	Comment	Reference
A	729	GLY	-	EXPRESSION TAG	UNP P08235
A	730	SER	-	EXPRESSION TAG	UNP P08235
A	810	LEU	SER	ENGINEERED	UNP P08235
A	910	ALA	CYS	ENGINEERED	UNP P08235
B	729	GLY	-	EXPRESSION TAG	UNP P08235
B	730	SER	-	EXPRESSION TAG	UNP P08235
B	810	LEU	SER	ENGINEERED	UNP P08235
B	910	ALA	CYS	ENGINEERED	UNP P08235
C	729	GLY	-	EXPRESSION TAG	UNP P08235
C	730	SER	-	EXPRESSION TAG	UNP P08235
C	810	LEU	SER	ENGINEERED	UNP P08235
C	910	ALA	CYS	ENGINEERED	UNP P08235
D	729	GLY	-	EXPRESSION TAG	UNP P08235
D	730	SER	-	EXPRESSION TAG	UNP P08235
D	810	LEU	SER	ENGINEERED	UNP P08235
D	910	ALA	CYS	ENGINEERED	UNP P08235
E	729	GLY	-	EXPRESSION TAG	UNP P08235

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Chain	Residue	Modelled	Actual	Comment	Reference
E	730	SER	-	EXPRESSION TAG	UNP P08235
E	810	LEU	SER	ENGINEERED	UNP P08235
E	910	ALA	CYS	ENGINEERED	UNP P08235
F	729	GLY	-	EXPRESSION TAG	UNP P08235
F	730	SER	-	EXPRESSION TAG	UNP P08235
F	810	LEU	SER	ENGINEERED	UNP P08235
F	910	ALA	CYS	ENGINEERED	UNP P08235

- Molecule 2 is SPIRONOLACTONE (three-letter code: SNL) (formula: $C_{24}H_{32}O_4S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			29	24	4	1		
2	B	1	Total	C	O	S	0	0
			29	24	4	1		
2	C	1	Total	C	O	S	0	0
			29	24	4	1		
2	D	1	Total	C	O	S	0	0
			29	24	4	1		
2	E	1	Total	C	O	S	0	0
			29	24	4	1		
2	F	1	Total	C	O	S	0	0
			29	24	4	1		

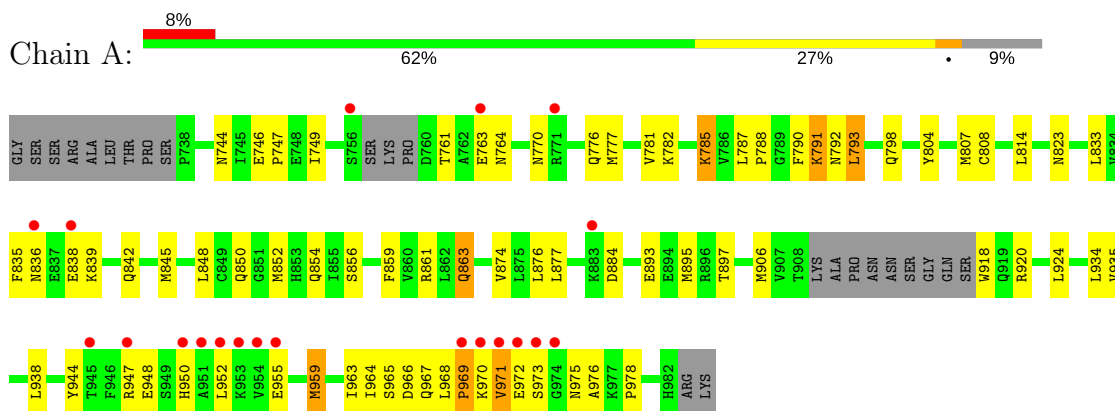
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	54	Total 54	O 54	0	0
3	B	53	Total 53	O 53	0	0
3	C	72	Total 72	O 72	0	0
3	D	66	Total 66	O 66	0	0
3	E	34	Total 34	O 34	0	0
3	F	60	Total 60	O 60	0	0

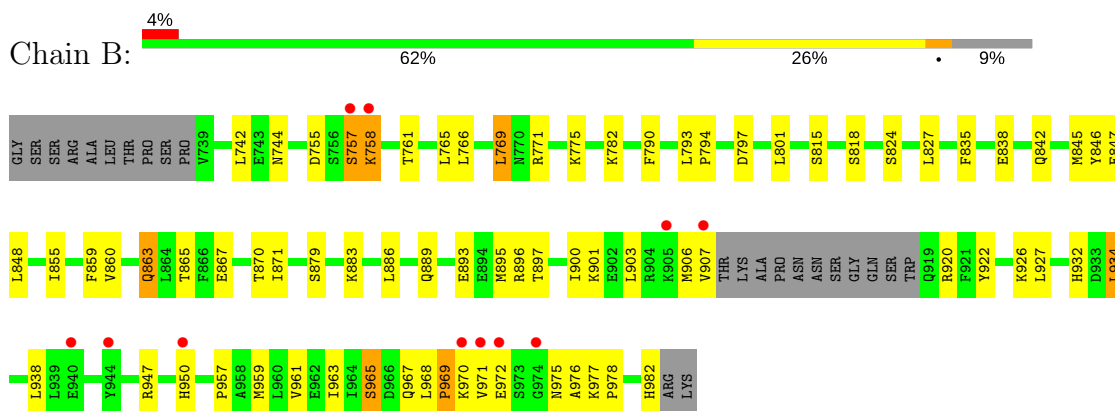
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

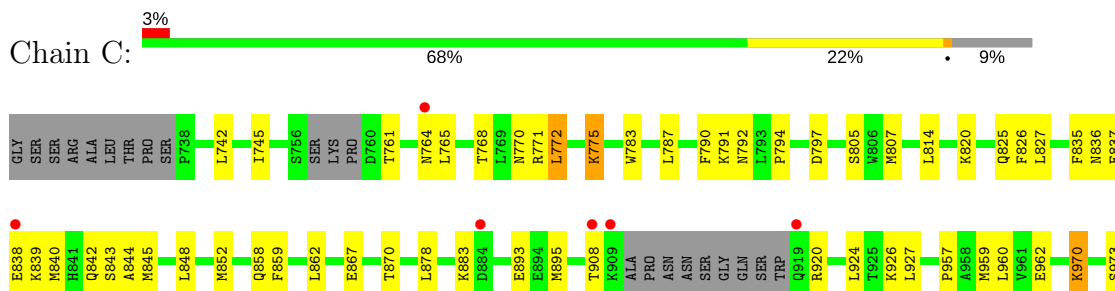
• Molecule 1: Mineralocorticoid receptor

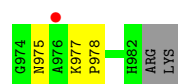


• Molecule 1: Mineralocorticoid receptor

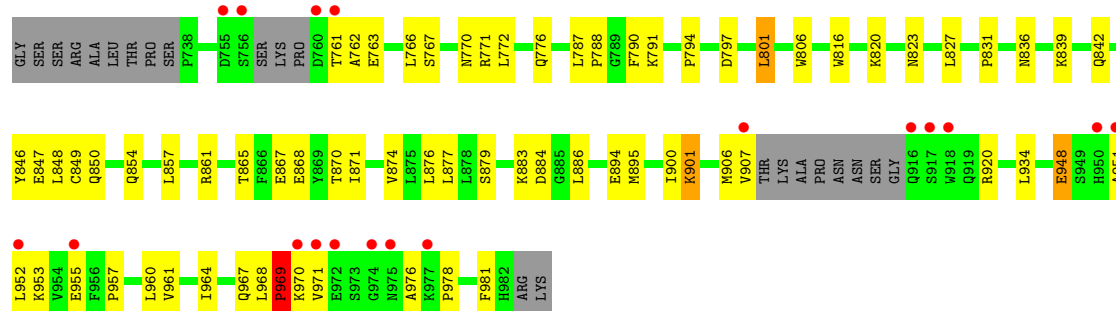


• Molecule 1: Mineralocorticoid receptor

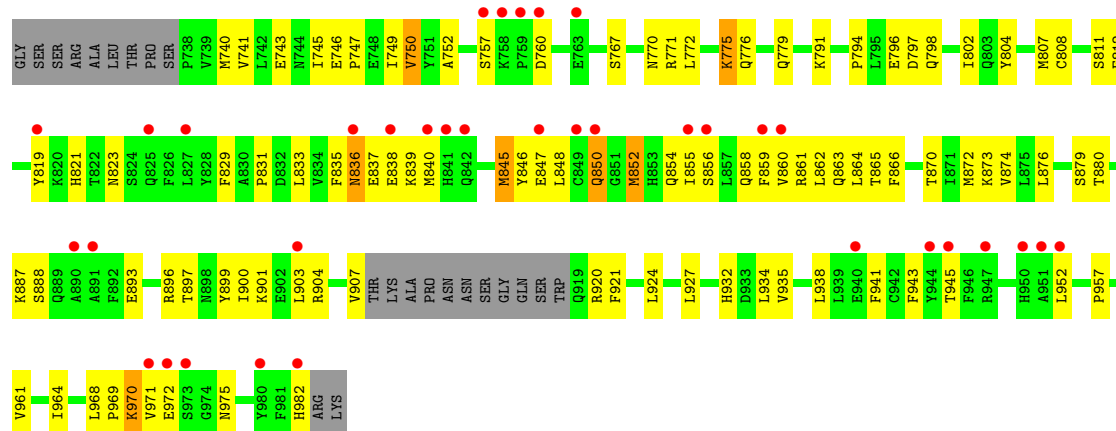




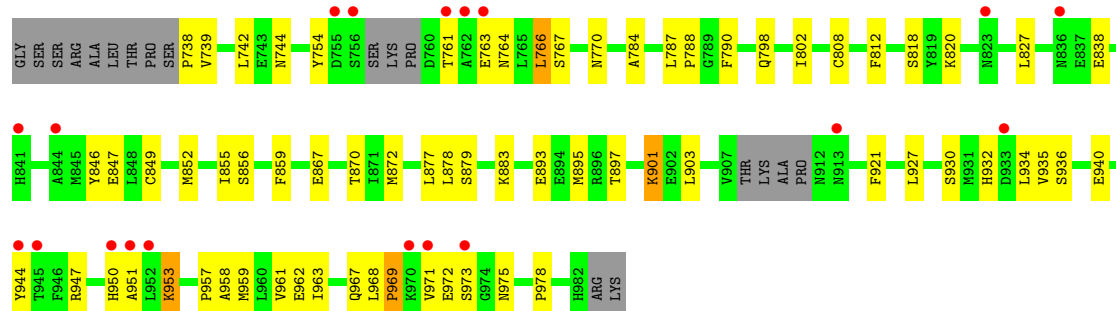
• Molecule 1: Mineralocorticoid receptor



• Molecule 1: Mineralocorticoid receptor



• Molecule 1: Mineralocorticoid receptor



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	122.20Å 122.20Å 91.81Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	14.92 – 2.29 14.92 – 2.29	Depositor EDS
% Data completeness (in resolution range)	91.2 (14.92-2.29) 91.3 (14.92-2.29)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.240 , 0.263 0.239 , 0.262	Depositor DCC
R_{free} test set	3220 reflections (5.12%)	DCC
Wilson B-factor (Å ²)	39.0	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.014 for -h,-k,l 0.034 for h,-h-k,-l 0.017 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12016	wwPDB-VP
Average B, all atoms (Å ²)	44.0	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 33.32 % 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 8.1530e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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: SNL

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	0.38	0/1948	0.55	0/2636
1	B	0.39	0/1960	0.56	0/2647
1	C	0.42	0/1956	0.59	0/2641
1	D	0.40	0/1963	0.60	0/2651
1	E	0.40	0/1956	0.58	0/2643
1	F	0.36	0/1984	0.54	0/2680
All	All	0.39	0/11767	0.57	0/15898

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1903	0	1887	62	0
1	B	1916	0	1929	64	0
1	C	1913	0	1920	38	0
1	D	1919	0	1921	56	0
1	E	1912	0	1919	75	0
1	F	1940	0	1932	56	0
2	A	29	0	32	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	29	0	32	1	0
2	C	29	0	32	6	0
2	D	29	0	32	4	0
2	E	29	0	32	6	0
2	F	29	0	32	10	0
3	A	54	0	0	2	0
3	B	53	0	0	1	0
3	C	72	0	0	1	0
3	D	66	0	0	2	0
3	E	34	0	0	3	0
3	F	60	0	0	3	0
All	All	12016	0	11700	359	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 15.

The worst 5 of 359 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)
2:F:6001:SNL:C24	2:F:6001:SNL:C23	1.74	1.65
2:F:6001:SNL:C22	2:F:6001:SNL:S61	2.04	1.44
2:C:3001:SNL:C22	2:C:3001:SNL:S61	2.08	1.39
1:A:852:MET:CE	1:A:934:LEU:HD23	1.58	1.31
1:A:852:MET:HE1	1:A:934:LEU:CD2	1.65	1.25

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	227/256 (89%)	214 (94%)	9 (4%)	4 (2%)	10 9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	229/256 (90%)	217 (95%)	10 (4%)	2 (1%)	20	23
1	C	227/256 (89%)	217 (96%)	9 (4%)	1 (0%)	38	47
1	D	228/256 (89%)	214 (94%)	13 (6%)	1 (0%)	38	47
1	E	230/256 (90%)	211 (92%)	18 (8%)	1 (0%)	38	47
1	F	232/256 (91%)	210 (90%)	19 (8%)	3 (1%)	14	14
All	All	1373/1536 (89%)	1283 (93%)	78 (6%)	12 (1%)	20	23

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	969	PRO
1	C	908	THR
1	F	969	PRO
1	F	973	SER
1	A	969	PRO

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	210/234 (90%)	201 (96%)	9 (4%)	33	45
1	B	215/234 (92%)	202 (94%)	13 (6%)	22	30
1	C	214/234 (92%)	202 (94%)	12 (6%)	25	33
1	D	214/234 (92%)	202 (94%)	12 (6%)	25	33
1	E	214/234 (92%)	197 (92%)	17 (8%)	14	18
1	F	216/234 (92%)	206 (95%)	10 (5%)	31	42
All	All	1283/1404 (91%)	1210 (94%)	73 (6%)	24	32

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	973	SER

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Mol	Chain	Res	Type
1	D	901	LYS
1	F	879	SER
1	D	842	GLN
1	D	934	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	825	GLN
1	D	975	ASN
1	F	854	GLN
1	D	850	GLN
1	E	798	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

6 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
2	SNL	A	1001	-	32,33,33	4.05	18 (56%)	48,54,54	2.16	14 (29%)
2	SNL	B	2001	-	32,33,33	4.82	21 (65%)	48,54,54	2.67	18 (37%)
2	SNL	C	3001	-	32,33,33	5.60	25 (78%)	48,54,54	2.27	14 (29%)
2	SNL	D	4001	-	32,33,33	4.84	19 (59%)	48,54,54	2.53	16 (33%)
2	SNL	E	5001	-	32,33,33	4.42	20 (62%)	48,54,54	2.30	12 (25%)
2	SNL	F	6001	-	32,33,33	5.56	21 (65%)	48,54,54	1.99	14 (29%)

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
2	SNL	A	1001	-	-	0/4/80/80	0/5/5/5
2	SNL	B	2001	-	-	0/4/80/80	0/5/5/5
2	SNL	C	3001	-	-	0/4/80/80	0/5/5/5
2	SNL	D	4001	-	-	0/4/80/80	0/5/5/5
2	SNL	E	5001	-	-	0/4/80/80	0/5/5/5
2	SNL	F	6001	-	-	0/4/80/80	0/5/5/5

The worst 5 of 124 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2001	SNL	O58-C9	-5.81	1.38	1.47
2	B	2001	SNL	C21-C22	-5.72	1.45	1.53
2	D	4001	SNL	C21-C22	-4.93	1.46	1.53
2	F	6001	SNL	C4-C3	-4.40	1.43	1.53
2	D	4001	SNL	O58-C9	-3.69	1.41	1.47

The worst 5 of 88 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	4001	SNL	O58-C9-C8	-7.17	101.65	109.34
2	E	5001	SNL	O59-C16-S61	-6.20	117.93	122.99
2	B	2001	SNL	O59-C16-S61	-5.84	118.22	122.99
2	C	3001	SNL	C4-C5-C9	-5.79	114.30	117.82
2	D	4001	SNL	C9-C5-C6	-5.16	95.02	99.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	SNL	3	0
2	B	2001	SNL	1	0
2	C	3001	SNL	6	0
2	D	4001	SNL	4	0
2	E	5001	SNL	6	0
2	F	6001	SNL	10	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, 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(Å ²)	Q<0.9
1	A	233/256 (91%)	0.39	20 (8%) 11 16	23, 41, 69, 82	0
1	B	233/256 (91%)	0.28	11 (4%) 32 39	24, 40, 58, 71	0
1	C	233/256 (91%)	0.16	7 (3%) 51 58	20, 37, 60, 71	0
1	D	234/256 (91%)	0.33	18 (7%) 14 19	20, 39, 71, 86	0
1	E	234/256 (91%)	0.82	35 (14%) 3 4	22, 57, 78, 82	0
1	F	238/256 (92%)	0.46	19 (7%) 13 17	23, 43, 75, 79	0
All	All	1405/1536 (91%)	0.41	110 (7%) 14 19	20, 41, 73, 86	0

The worst 5 of 110 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	951	ALA	7.5
1	D	951	ALA	6.4
1	E	951	ALA	6.3
1	B	970	LYS	6.3
1	E	760	ASP	6.1

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(Å ²)	Q<0.9
2	SNL	D	4001	29/29	0.92	0.15	0.41	22,27,29,30	0
2	SNL	B	2001	29/29	0.95	0.13	0.00	19,21,23,24	0
2	SNL	A	1001	29/29	0.95	0.14	-0.17	25,29,31,32	0
2	SNL	E	5001	29/29	0.92	0.16	-0.22	42,43,45,47	0
2	SNL	F	6001	29/29	0.93	0.13	-0.64	29,34,38,40	0
2	SNL	C	3001	29/29	0.96	0.11	-1.02	18,23,25,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.